

LABORATORY DIRECTED RESEARCH AND DEVELOPMENT

Expanding Professional Horizons

*Collaboration, Challenge, and
Continuity through LDRD*

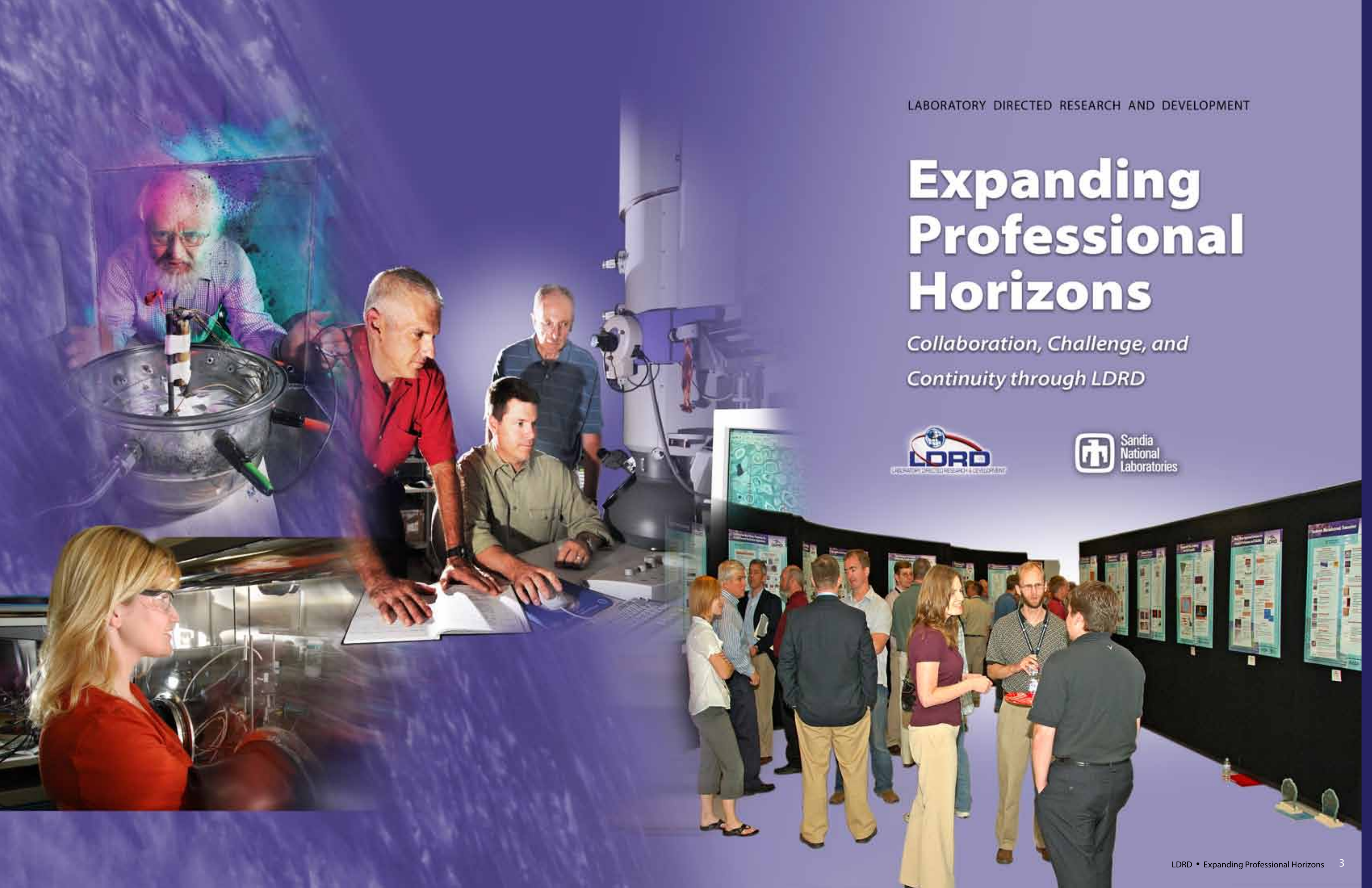


Sandia
National
Laboratories

LABORATORY DIRECTED RESEARCH AND DEVELOPMENT

Expanding Professional Horizons

*Collaboration, Challenge, and
Continuity through LDRD*



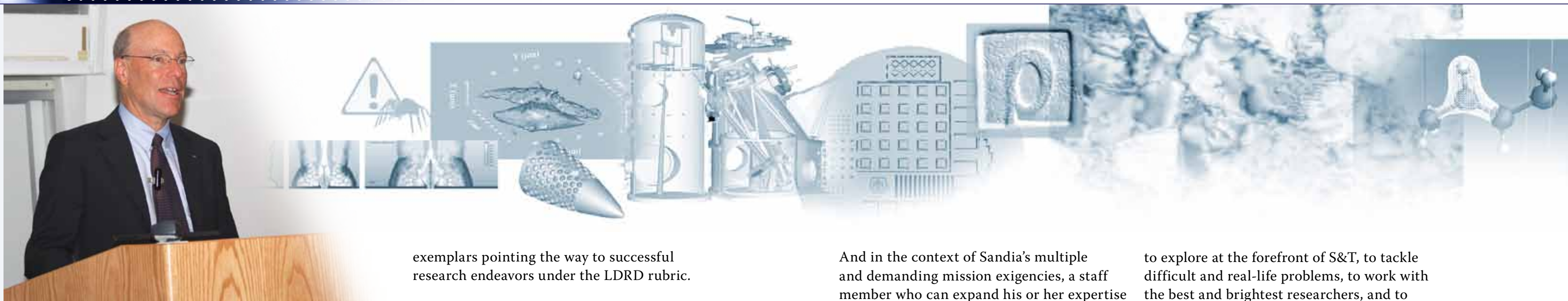


Expanding Professional Horizons

Contents

Overview	6
Early-Career	8
Mid-Career	22
Late-Career	36

For further information, contact:
Henry R. Westrich
LDRD Program Manager
hrwestr@sandia.gov
505-844-9092



Overview

Rick Stulen, VP Science, Technology and Engineering, and Chief Technology Officer, Sandia National Laboratories

The impact of the Laboratory Directed Research and Development (LDRD) program on staff at Sandia is felt in numerous ways and at all levels of career development, from the individual who comes to Sandia as a Truman Fellow, funded for three-years of innovative research, through the late-career staff member who, along the way, has mentored and guided earlier-career staff in diverse ways.

This publication highlights a myriad of ways in which the Sandia LDRD Program has nurtured staff development for individuals at different stages of their careers. These 20 stories are merely an exemplary subset, and there are clearly other success stories, untold. In addition to staff development, what emerges from these stories is also the creative energy that underlies the problem-solving brilliance and collaboration that is central to Sandia LDRD as its researchers seek technical solutions to national security challenges. These individual and collective characteristics are certainly worth noting and perhaps even worth emulating as

exemplars pointing the way to successful research endeavors under the LDRD rubric.

Perhaps most importantly, LDRD is a mechanism that has created a vast number of cross-cultural partnerships across the laboratory. Cross-center, cross-division, or even cross-institution, scientists and engineers of greatly differing skill-sets and backgrounds have been able to forge partnerships in pursuit of a common goal — to discover new principles or applications thereof, create new problem-solving approaches or technologies, or prove concepts or immature technologies by resolving unknowns. Because science has become so multidisciplinary, with common underpinnings to problems that were once viewed as germane only to specific and bounded disciplines, it stands to reason that challenges at the leading edge of science require cooperative assemblages of scientists and engineers. For example, to seriously approach solutions to optimization of certain renewable energy sources within the context of global climate change requires experts in chemical thermodynamics, cell and molecular biology, electrical and mechanical engineering, microfabrication, computational modeling, climatology, and perhaps other areas as well. It is unlikely that this repository of knowledge and understanding — in depth — lies within the grasp of a single individual. But at a national laboratory with the breadth and depth of the research staff at Sandia, a partnership of individuals in these fields is not only possible, but has been demonstrated in multiple instances during LDRD projects.

And in the context of Sandia's multiple and demanding mission exigencies, a staff member who can expand his or her expertise into fields related or complementary to his/her central area of expertise, becomes that much more valuable in the context of forging such collaborative teams, both in direct programmatic work, and in the partnerships often required to pursue the leading-edge research funded through LDRD. This will often involve some degree or form of mentoring by more-experienced staff members. In addition, such expansion of personal expertise is often facilitated by partnerships with researchers from academia, industry or other government labs, a feature of the LDRD program that is crucial to recognize and to nurture. Although great ideas are sometimes the product of single individuals, it is perhaps more often the case that the development of truly innovative science and technology flows from the collaboration of researchers who are all working at the leading-edge of a challenge, often from different but complementary directions.

There is also ample evidence that LDRD has attracted high-quality staff to Sandia, who might otherwise not have come. From the young scientist offered a position at MIT — who instead chose the early-career flexibility offered by his colleagues' and his own LDRD research — to the graduate student, unaware of Sandia's position in the national landscape and apprised of exciting Sandia research by a friend or colleague, LDRD is a critical recruiting resource, because there is freedom

to explore at the forefront of S&T, to tackle difficult and real-life problems, to work with the best and brightest researchers, and to have impact. Scholarly publications are often the immediate outcome of such research efforts, and this flow of scholarly information in the peer-reviewed literature and at national and international meetings provides Sandia and its LDRD program with critical exposure for its researchers and vetting of its scientific or technical contributions. It is also an invaluable recruiting tool — a window into exciting LDRD research for the young scientist deciding on a career path.

In parallel with the external transparency that scholarly publication confers, and given the track record of positive interdisciplinary collaborations, LDRD Program management has been working to encourage all Sandia staff to form strategic partnerships both within and outside Sandia. Most importantly, the program continues to move in a direction whereby staff understand that LDRD welcomes projects, which because of their ingenuity and innovative disposition, incur risk. To allay this risk-aversion disposition in staff members is critical to nurturing great ideas and potentially boundary-breaching and status-quo-transcending research. Risk is opportunity! These creative leaps into a more-secure national future are, indeed, the reason that Congress funded LDRD at DOE national laboratories. And in the face of the immense current challenges to national security, encouraging risk-taking in developing creative research strategies to address those challenges is a crucial aspect of Sandia LDRD.

EARLY-CAREER

Risk as Opportunity for Collaboration

Still Amazed by the Possibilities

Meredith Anderson

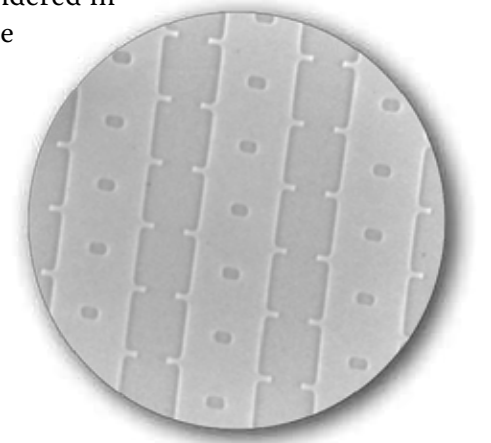
“Orphaned” by the decision of her Ph.D. thesis advisor at Carnegie-Mellon University (CMU) to accept a position in industry, Meredith Anderson returned to Sandia — where she had previously spent a summer month — to complete her graduate studies under the tutelage of Sandian Brian Swartzentruber and a committee back at CMU. “It was a better way to do it,” she reminisces, considering herself fortunate to have been funded as a part of a DOE basic energy sciences grant.

After defending her dissertation in 2004, Anderson stayed on as a postdoctoral (postdoc) researcher, and her mind quickly began to form bridges. If the imaging techniques she had studied as a graduate student had been useful in that context, then why not microelectronics? *I might as well*, she thought — the attitudinal disposition of the academician to seek funding sources well-ingrained in her psyche. “I thought it was a longshot,” she says of the LDRD idea she decided to submit, “but they said they wanted high risk.” Convinced of the technical merit of her idea, Meredith found herself “still amazed” by what had become possible in the field of materials imaging. For example, based on the quantum mechanical phenomenon of electron tunneling, the Nobel Prize-winning invention of scanning tunneling microscopy had allowed researchers to image surfaces at the atomic level with a resolution of 0.1 nm, an astounding capability for microscopists satisfied with electron microscope resolutions of perhaps 5 nm, prior to the discovery.

For Meredith Anderson, such capabilities are motivating, keeping the work “exciting” and “fun.” Hence, despite her skepticism, her first attempt at LDRD funding achieved success to her great, but pleasant, surprise.

And as Anderson plunged into the research, she discovered — as many researchers do — a two-edged sword. One edge cut cleanly and precisely, confirming the exciting propositions tendered in the prospectus, while the other edge raised as many question as it answered, provoking some confusion. This didn’t stop Anderson, for she had already learned the value of consultation and collaboration. Turning to senior scientist, Ed Cole, still an active researcher in this area of characterizing microelectronics defects provoked by various factors, Anderson found him interested not only in her LDRD project, but also in eliciting her participation on some of his own work.

Despite these positive outcomes in eliciting senior collaboration, Anderson was still a postdoc leading an LDRD project, and in light of this situation, her management hired her as a limited-term staff member. Centered in the nanosciences and microsystems area, Anderson believes that her first LDRD project benefitted from its “good timing,” in the sense that Sandia’s Microsystems and Engineering Sciences Applications (MESA) project was approaching completion during this same period. As such, as its microelectronics/optoelectronics facilities became operational, Anderson was heavily involved in contributing to the team effort that brought the facilities fully on line. “I know I did a good job at my parts of the work,” she recalls, this assessment supported by a suggestion from Cole that she should consider writing a second LDRD proposal.



A high-resolution micrograph of silicon, capable of distinguishing p-doped regions. (lighter areas) from n-doped regions (darker areas).

“*I thought it was a longshot . . . but they said they wanted high risk . . . It gave me flexibility to be able to explore the possibilities.*”

Anderson had found a mentor and a team of collaborators from several organizations, her microcopy results showing a high potential for her work to have significant impact in imaging details of microelectronics components for a variety of Sandia mission applications. The first LDRD project, a more fundamental and exploratory incursion into teasing out what might be possible, a proof of concept, set the stage for the second proposal, which approached the imaging possibilities from the more applied angle, with which she had become more familiar in her interactions with the various staff members who had participated in the stand-up of MESA. “It gave me the flexibility to be able to explore the possibilities,” Anderson comments about her first LDRD project. And at about the same time period as the funding of her second LDRD proposal, also came her hiring as a regular staff member, a correlation that Anderson perceives as connected if not causally related — at least in the sense that the quality of her ideas and research and her willingness and ability to forge collaborations were exemplary of her current and potential future value to her organization and the Laboratories.

Anderson continues to make use of the richness of expertise and cross-center collaborations possible at Sandia. Based on the exhibited potential of imaging techniques such as low-energy electron microscopy (LEEM), she has consulted with other teams of Sandia scientists who might benefit from its capabilities. “It’s really great to have these meetings; it’s maybe a few years down the road that you’ll see the effect,” she notes with a sense of anticipation, expressing the belief

that Sandia’s richly variegated environment presents innumerable opportunities for creative collaboration. She exhibits an understated confidence that the capabilities that she is developing and validating with LDRD support will offer an important asset for microelectronics and optoelectronics researchers and developers in years to come.

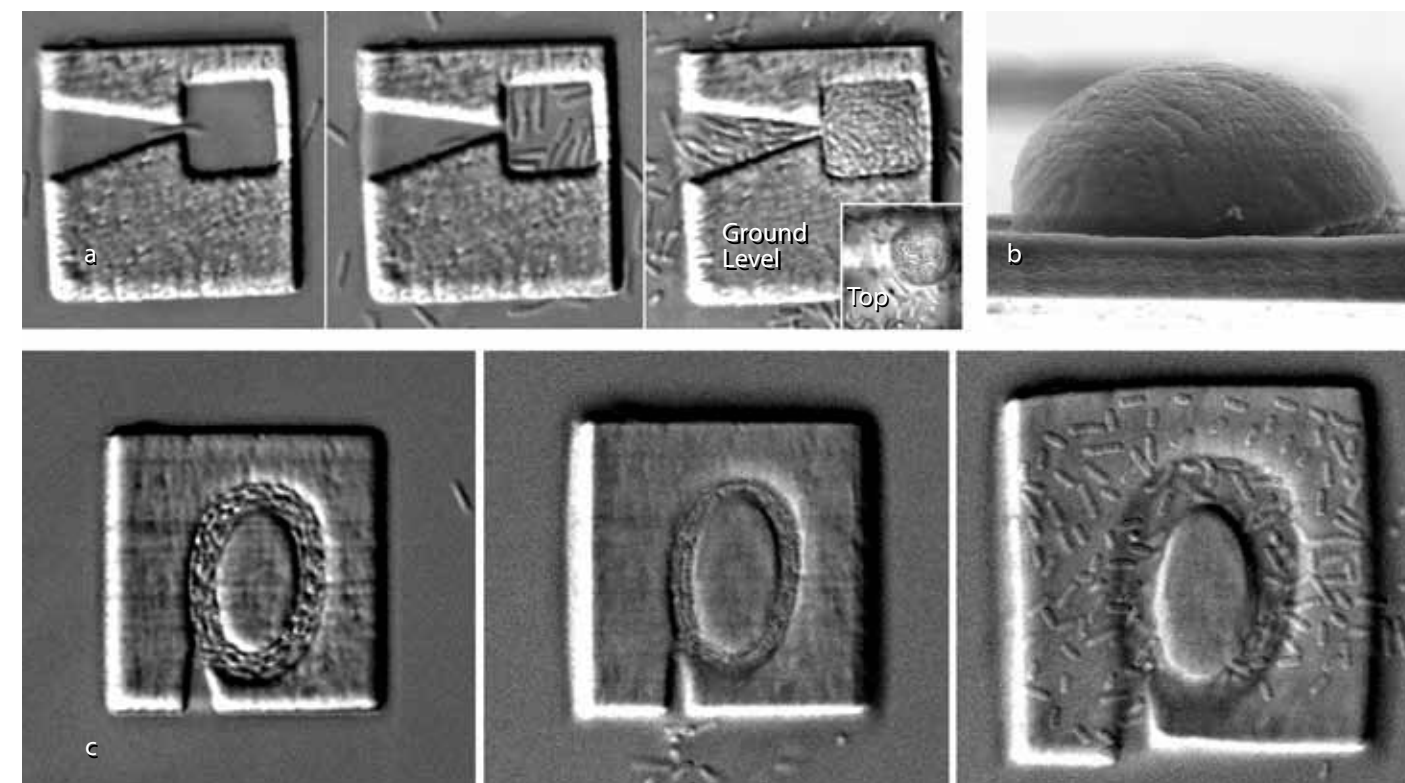
Finding a Mentor-Collaborator

Attuned to Serendipity

Bryan Kaehr

Describing this as “an exciting time to be at Sandia,” and himself as an individual “attuned to serendipity,” Truman Postdoctoral Fellow and Albuquerque native, Bryan Kaehr sees himself amid a burgeoning initiative at the interface of biology and nanotechnology. Bio-nano interdisciplinary research is, quite obviously, not only in-progress at the Laboratories, but it is also growing and attracting the attention and energies of creative young staff like Kaehr. These early-career individuals are not only coming to seek growth and career-development opportunities, but they are also bringing with them unique opportunities for this facet of Sandia LDRD-funded research efforts.

Although invited to present a seminar on his doctoral research that was, already, a bio-nano initiative, Bryan was, at first, somewhat daunted by the Truman announcement, which he perused on a bulletin-board flyer at the University of Texas (UT), Austin. It appeared from the flyer that the requirements bar for the fellowship was set rather high. But after a one-on-one meeting at which Jeff Brinker (page 38) encouraged him to apply, Kaehr recognized the opportunity to integrate his research with that of Brinker’s ingenious team and followed through, firmly believing that his unique protein lithography system could be



Creating dynamic cell enclosures by way of lithography of protein hydrogels enables the trapping of single bacterial cells (a, upper, left), followed by accumulation of colonies of cells (a, third panel, and c. left panel). Each cell is an elongated rod. (copyright 2008, National Academy of Sciences, USA; originally published in Kaehr, B. and J. Shear, *Proceedings of the National Academy of Sciences*, vol. 105, page 8850-8854, 2008).

of both great interest and great potential value to the Sandia research ongoing in this arena. Echoing the sentiments of other Truman applicants and awardees like Anatole von Lillienfeld (p. 17), Bryan was looking for a laboratory offering the freedom to pursue novelty, to investigate the leading-edge, in this instance, the leading edge of the leading edge, a multidisciplinary scientific field in its infancy. The Truman, and the associated LDRD-funded endeavors in Brinker’s group clearly presented such an opportunity.

Building a better micro-box for cells in which to live would be a completely pedestrian way to describe this work, but both the approaches and the questions posed extend far beyond such a mundane description. But both Kaehr and Brinker, his Sandia project manager, are approaching this nanomanipulation of microenvironments from slightly different angles. Kaehr had published his technique for

laser-light-based manipulation of proteins within a hydrogel matrix — so-called multiphoton lithography — one that allows him to create a diversity of nano and microenvironments that are manipulable by physical parameters such as pH (acidity) and temperature. But these environments are also biologically significant, because proteins are bionanomachines of various types (signalers, receivers, motors, and enzymes, for example). Thus, incorporation of living cells into such a nano-fabricated proteinaceous environment makes this a potentially interactive situation, in which the cells can interact with and remodel this light-fabricated structure.

Coming from his background as a materials scientist, nano-manipulating inorganic materials, Brinker, meanwhile

“*This is an exciting time to be at Sandia . . . a ripe place for biology.*”

has nonetheless pursued a parallel path in nano-constructing biologically compatible environments, in his case, a composite of inorganic silica and layered lipids (the “stuff” of biological membranes). Brinker’s team has demonstrated that living cells will interact with and actively manipulate the surrounding architecture.

Meanwhile, Kaehr has trapped and incubated living cells in micro-enclosures formed by his method. Hence, the marriage of these two approaches may logically open up a myriad of novel possibilities. At least two possible research pathways loom, one more immediate, the other more futuristic. More proximal are investigations into cell signaling, fundamental questions abounding in signaling pathways that appear to govern so-called quorum sensing in bacteria — by which a grouping of single-celled organisms appear to self-regulate as though they were a multicellular organism. Numerous signaling processes also await clarification in higher organisms, for example, the immune system, a “liquid, distributed brain,” representing a model system for study. More futuristic are intentions to utilize cells as modelers of nanomaterials; for example, one could envision a bacterial cell, yeast cell, or even a white blood cell becoming the creator of circuitry on a silicon communications chip. Once the stuff of science fiction, this design potential is now not only conceivable, but both Brinker’s and Kaehr’s systems provide rational routes to such eventual outcomes.

The fact that the two investigators are now working together rather than separately — one a distinguished Sandia staff member and distinguished UNM professor, the other an early-career scientist — is testament to the possibilities inherent in the LDRD program and the Truman fellowship. Kaehr speaks of Sandia as a “ripe place for biology.” In his amazement at the diversity and quality of science occurring here, he predicts that the Laboratories will develop more niches “for people like me.”

The Truman and the underpinning philosophy of the LDRD program is clearly a win-win for both Kaehr and Sandia. By offering freedom to pursue cutting-edge science in the company of astute, creative colleagues, the Laboratories attracted a young, creative researcher and potential future staff member, who brings with him an innovative approach that both complements and supplements ongoing work in this remarkable new field. Although Kaehr may view his application for the Truman as serendipitous, Brinker’s active outreach to creative young scientists, under the auspices of the LDRD program is also exemplary of a very wise investment by the DOE and Sandia management in a LDRD program that makes such collaborative cutting-edge science a genuine possibility.

Creative Opportunity and Strong Leadership

Choosing the Creativity Option Jacques Hung Loui

“We wish we had a program like LDRD to offer you,” said the voice on Jacques Loui’s cell phone. The phone call was from a manager at MIT’s Lincoln Laboratories, and the voice had just offered him a highly coveted prize for any graduating Ph.D.— the opportunity to conduct research as a staff member at one of the premier physical science laboratories in the world.

But, while standing in Boston’s Logan Airport, about to board his return flight after his MIT interview and a few weeks prior to that affirmational phone call from MIT, Jacques had received what would turn out to be an even more significant call from Sandia Vice-president and Chief Technology Officer, Rick Stulen, offering him — through the LDRD Program — a President Harry S. Truman Fellowship. And it was that call from Stulen that took precedence,

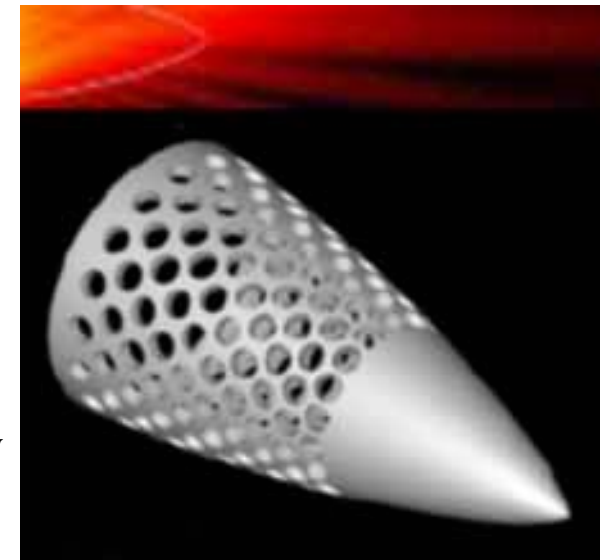
steered the course of Jacques’s career. For, as Jacques would explain to his MIT solicitor, his priority was creativity — in order for him to blossom as a scientist, he felt strongly that creative space offered by the Truman fellowship, the LDRD program, and the broad scope of Sandia research efforts would best address his aspirations. He had taken extra time in his doctoral research so that he could pursue the triad of experimental, numerical, and theoretical approaches to electromagnetic radiation scattering from complex objects, and he felt that the Truman Fellowship would enable him to continue on all fronts, giving him “freedom in deciding an area of pursuit.”

The MIT caller sweetened the deal, offering a signing bonus. But for Jacques, Sandia was the “best-kept secret” in US science; the breadth of globally and nationally significant research funded under the LDRD umbrella had already played its magic on his thinking. He would pursue the path that allowed him to create, innovate, and collaborate, while charting a course into the waters of national security in the person of Sandia’s synthetic aperture radar (SAR) technology. Most important to Jacques were the bonds he rapidly forged with his peers. He immediately sensed that his Sandia mentor Billy Brock, appreciated his work, and was fantastically encouraging, both scientifically and personally. He exemplified, “not only a mentor, but a leader” within “a culture of mutual respect, trust, and engineering excellence at Sandia.”

This culture of excellence and mutual respect has convinced Jacques that he has found a home at Sandia. His Truman LDRD involved a creative method for controlling electromagnetic radiation (light) by designing metal surfaces with periodic arrays of computationally designed “cells” — essentially elaborately configured apertures — to allow active control of signals for diverse applications — sensors,

antennas, and lenses, to name just a few. He credits LDRD and the support by Brock and manager Kurt Sorensen for making “every possible effort” in his behalf, ensuring that he was “never isolated.” As his Truman fellowship entered its final year, Jacques pitched a follow-up idea to Sorensen — after discussing it with several of his peers — and was rewarded as a member of an LDRD-funded team, for which, as a still-Truman Fellow, he could not serve as principal investigator (PI). But this allowed Jacques to pull together a collaboration with a team, whose PI, Bernd Strassner, has become not simply a fellow-scientist whose ideas resonate with Jacques’, but also a friend and an officemate. With distinct national security implications, the research — in the arena of control of electromagnetic radiation — is, in principle, related to Jacques’ Truman fellowship work.

Now a full-fledged, cleared staff member, Jacques will be finishing his executive MBA at the University of New Mexico, this year, and is looking toward a future in realms of greater responsibility at Sandia. “To me, education is life,” says this budding young



Original design by Jacques Loui of a metal cone with periodic arrays of cells for controlling electromagnetic radiation. © Hung Loui 2005

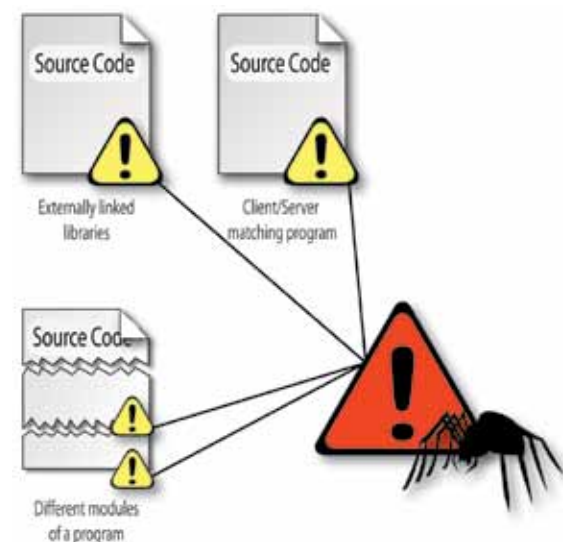
“... a culture of mutual respect, trust, and engineering excellence at Sandia.”

scientist, born near the Gobi desert. “Great leaders can see the goals of the people around them,” Jacques observes, and even at this early phase of his own career, it appears that he has the makings of leadership, which the LDRD program is nurturing.

Teamwork in Addressing National Security Challenges

Competition Driving Innovation Jonathan Margulies

Becoming an important, trusted young staff member at a place he’d “never even heard of”: This outcome for Jonathan Margulies reflects the broad reach and great accomplishments of Sandia and Sandia LDRD, even if that reach is frequently “silent” — or, rather, concealed within the experience of individuals. In this instance, and “by luck,” Jonathan’s roommate at Cornell had worked, as a student, for a scant six weeks at Sandia under Joselyn Gallegos; yet even that



A representation of the creation of a dangerous vulnerability through combination of disparate, seemingly innocuous features in various parts of source code, or various parts of a system.

short stint had been sufficient to convince the roommate that it was an interesting, productive, and high-quality environment.

Taking the initiative as he approached the completion of his Masters in Computer Science, Jonathan investigated, and indeed found himself recruited by Gallegos. During his visit/interview process, he discovered common interests and attitudes with manager Bob Hutchinson, on both a personal and a professional level. With the opportunity to work in either California or Albuquerque, Jonathan chose the latter, despite other personal preferences, and to a great extent based upon his perception of the interpersonal potential he saw through Hutchinson and other members of his prospective team.

Ultimately, the payoff was quite worthwhile, Margulies finding himself amid “exciting research opportunities” within “a vibrant, exciting place to work.” The “bigger laboratory with a smaller profile” had suddenly opened up before him, displaying broad vistas of possibility, possibilities that were intimately tied to LDRD funding to examine fundamental aspects of information science, as well as to participate in the development of new analytical tools. What may sound like an overall simple challenge — protect critical information resources — can actually be astoundingly complex, when one considers the intricacies of that challenge. And aside from the discovery and implementation of mechanisms to accomplish that protective initiative, there is the accompanying, and perhaps even more daunting challenge of how best to assess the results of one’s implementations.

Jonathan’s dual skills as computer scientist and writer quickly made him an invaluable asset, as his programmatic duties in code development were supplemented by his documentation of both his own work and that of colleagues. In this role, he was favored with a broad view of the research and development

activity in his group and organization. It also permitted him to quickly develop a network of trusted relationships.

These skills and developmental potential soon came into play as Sandia Laboratory Fellow Jim Gosler decided to increase the concentration of resources into this arena of information protection, and he called for ideas worthy of LDRD funding. Through Bob Hutchinson, a competitive set of interviews ensued to establish project leadership. Jonathan was chosen to lead one of two teams that would compete and co-evolve, and, ultimately, he became the LDRD’s principal investigator. Initially a short, late-start project, the work flourished, and within the circle of relationship that he had developed, Margulies and several colleagues submitted a second proposal that LDRD funded for a two-year timeframe. “Competition drives innovation,” Margulies reflects, but there was also “a real camaraderie within that competitive atmosphere.”

Within the context of this LDRD work, the team and the group has engaged a number of summer interns, and Jonathan is amazed at the talent. “There’s a great pipeline of young talent available to Sandia,” he reflects. Remarkably, in a group where over half the technical staff members are under the age of 30, the odds are that this critical area of Sandia mission work will continue to be stimulated to innovation by fresh young minds. However, in reflecting on the competitive process engendering the LDRD success, Margulies emphasizes that each of the relatively young teams in the competition had an experienced senior staff member as an advisor/mentor. In a sense, the situation reveals an orderly generational transition, whereby in a field such as information science — which expands daily, by leaps and bounds — knowledge turnover must be accompanied by an infusion of new talent that both informs and is informed by existing, experienced staff. With the discipline, by definition, always poised at the leading edge, LDRD becomes a natural vehicle for facilitating not only steps forward at that leading edge, but

also the intergenerational collaborations that are critical to creative risk-taking.

Jonathan believes that “LDRD has inspired our work for customers to new heights.” An important guiding idea is the understanding that seemingly innocuous bits of source code in different parts of a system can sometimes combine to create dangerous cyber-vulnerabilities. Margulies sees Sandia’s work in unearthing, assessing and protecting against such critical information vulnerabilities — particularly in the form of a Sandia-developed training tool — as ultimately transferrable to and hopefully adopted by every federally funded research and development center (FFRDC).

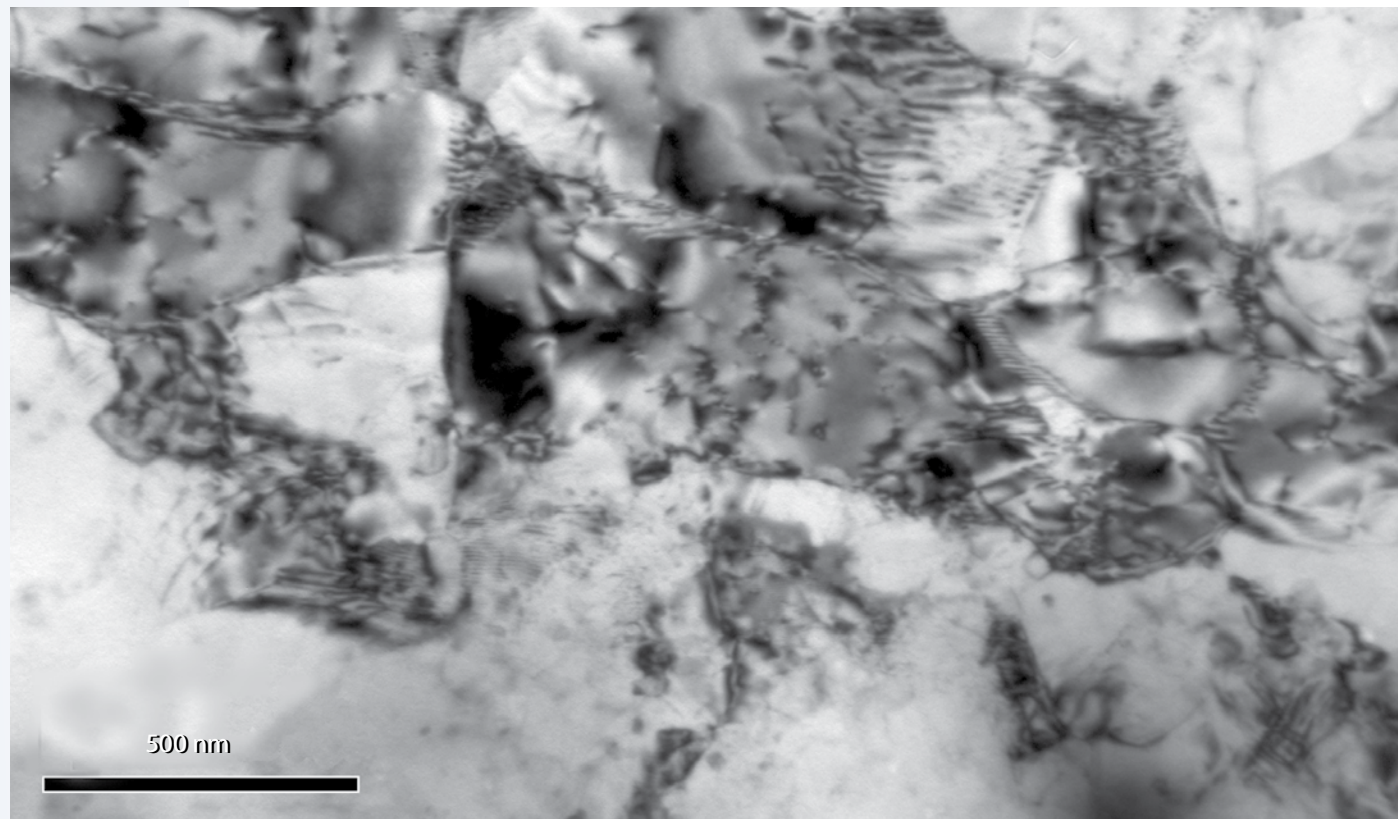
“The reason people come to us for cyber is that we have more-innovative research than our competitors, and that’s LDRD.” Clearly that attitude has both firmly engaged Jonathan Margulies’ talents and shown him a path to further developing them and sharing them with a broader Federal constituency.

Networking to Expand Capabilities

Encouraged to Try Again Chris San Marchi

With an MIT education and research experiences in metal foams and intermetallics, Chris San Marchi was just a bit out of his comfort zone when he accepted a job at Sandia that brought him responsibility for metal

“The reason people come to us for cyber is that we have more-innovative research than our competitors, and that’s LDRD.”



Transmission electron micrograph of a nanostructured aluminum-magnesium alloy.

forging. Yet his experience with alloys and his familiarization with the mission needs of his organization provoked his mind to consider approaches that might both challenge his scientific acumen and serve Sandia's multiple missions in gas transfer systems, both military- and civilian-related.

So after a few years at the Laboratories, Chris' experience with aluminum alloys led him to submit an LDRD proposal. And although the creative idea invited a proposal, the proposal itself did not succeed in gaining funding. However, as part of the possible feedback mechanisms structured into the LDRD process, the selection committee encouraged him that the idea was sound and worthy, and it encouraged him to reapply.

"I was pleasantly surprised and somewhat overwhelmed," says Chris of that second attempt, successful in securing three-year project funding to experimentally investigate and model the fundamental properties of

nanostructured aluminum alloys. San Marchi pressed forward in an environment where he had not yet had either the longevity or the time to become associated with a significant fraction of his peers. But as the mother of invention, necessity, in this instance, fueled collaboration. "People knew we had an LDRD program," he relates, in recalling how the funding gave him local visibility.

"It gave me the opportunity to interact with other staff on tough scientific problems," San Marchi comments on a common theme pervading LDRD funding recipients, namely an encouragement to collaboration. In an atmosphere such as Sandia, the program has particular value, particular strength. For in taking on a research responsibility, a staff member knows that gaps in his or her expertise can be readily filled through collaboration. As echoed by others (p. 25), there are so many Ph.D.-level experts to be found at Sandia, that a principal investigator (PI) with LDRD funding would be foolish to

not tap such a rich font in seeking to fill those expertise gaps. And science has become so multidisciplinary and so complex with the continual addition of scientific knowledge, that to approach the type of vanguard research that characterizes LDRD is quite likely to entail knowledge from related disciplines, of which no one individual is likely to have mastery.

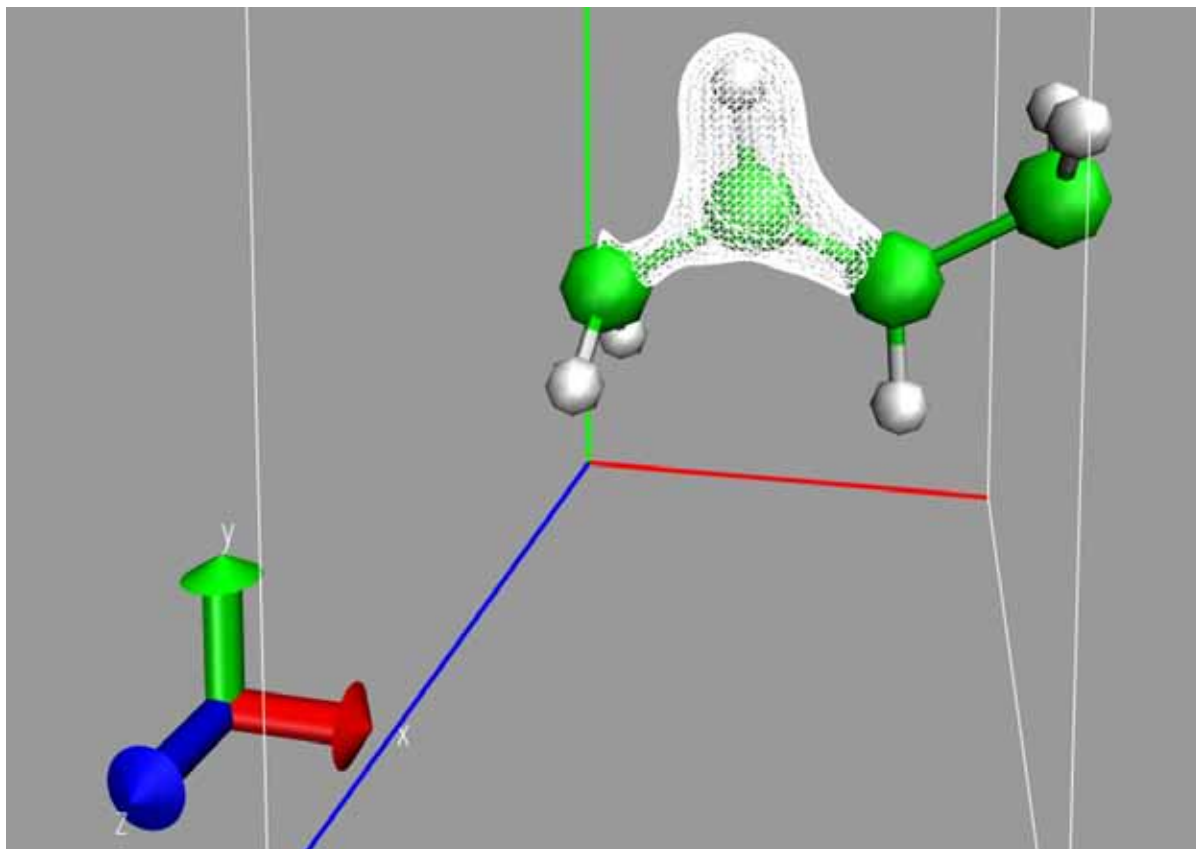
So it was that San Marchi developed relationships that not only assisted his own LDRD interrogation of nanostructured metal alloys, but also brought him into contact with both microscopists and other metallurgists at Sandia, who reciprocally sought his expertise on their projects — this cross-fertilization both within and across disciplines another common theme facilitating career development and enrichment for LDRD PIs and staff.

Nanostructured aluminum alloys show some remarkable mechanical properties. For example, they exhibit strength that is two or more times greater than conventional solid-solution strengthened aluminum alloys; and their nanostructure remains intact at very high temperatures, up to 80% of the melting point of the alloy, an unusual characteristic for nanostructured alloys. There are two important spinoffs of these properties. The first implication is obviously for structural applications, that is the fabrication of lighter vehicles and aircraft with greater cruising range, and moreover, that would be more-energy efficient to power. But second, preliminary studies suggest that these alloys are resistant to a phenomenon known as hydrogen-assisted fracture, in which hydrogen facilitates cracking — as it does in most structural steels. Since they appear resistant to hydrogen-assisted fracture at pressures up to 20,000 pounds per square inch (psi), nanostructured aluminum alloys are potentially valuable as containment materials for high-pressure storage of gaseous hydrogen for utilization in hydrogen fuel cells.

True to the project's LDRD roots, the issues that San Marchi and his co-workers pursued were fundamental: investigating the underlying structural and metallurgical underpinnings of the properties of these alloys; they pose the hypothesis that segregation of magnesium to the grain boundaries of nanostructured aluminum plays an important role in defining these unique properties.

“It gave me the opportunity to interact with other staff on tough scientific problems.”

San Marchi's work has "brought lots of industrial folks to Sandia," which San Marchi finds "really exciting and rewarding," and has brought external funding to his work. And of course, given that encouragement, Chris is grappling with two new LDRD ideas that would explore fundamental materials issues in the gas-transfer system arena, but with broad applicability to national energy security. This time, however, the process has taken on a slightly different shape, in that with co-workers already allied and potential collaborators identified, San Marchi has assembled a small team in each case. "I have some hope for this next LDRD," he reveals, despite the fact that he also regrets having not fulfilled all of his aspirations for the one just ended. But that admission frames a key personal aspect of LDRD PIs that also clarifies a contribution to their development as staff members at Sandia. When one has the wherewithal, the personal honesty, to understand that all has not been accomplished, that scientific and technical questions remain unresolved, and one is willing to push harder against those boundaries of scientific uncertainty, the reward can be great — not only for scientific knowledge itself and one's peers in the discipline, but for one's own personal integrity and capabilities as a scientist or engineer. Chris San Marchi appears to exemplify such integrity.



Quantum-mechanical probability distribution to predict the effect on the redox potential of a polymer due to annihilation of an Hydrogen atom.

Computational Potency to Model Engineering Solutions

An Inspiring Breadth of Science

O. Anatole von Lilienfeld-Toal

What does one do when faced with an engineering dilemma underpinned by the fundamental science of material properties? In the past, the only answer was to hypothesize a direction for scientific experimentation that might bring one closer to an engineering solution, then design an experiment to test the hypothesis. Hypothesize, test, evaluate outcome, repeat. And repeat and repeat and repeat, unless one is extremely brilliant or extremely fortunate.

But what if the engineering solution holds a key to improving a crisis such as the one facing our nation and the world in the area

of renewable energy and climate change?

The question then becomes, “is there a faster way to do this, by predicting the best course for experimentation?” Truman postdoctoral Fellow Anatole von Lilienfeld believes that better way involves computationally devising accurate chemical structure-materials property relationships through multiscale descriptions involving Ab Initio Molecular Dynamics.

For someone of his disposition, Sandia is “a very attractive place to be,” offering the opportunity to “collaborate with very capable scientists” to potentially “devise a software tool allowing us to routinely design valuable materials that actually get used.” For example, the Sandia solar-thermal tower employs a molten salt to store thermal energy from sunlight, later releasing it to drive a mechanical engine that turns an electrical generator, thus converting sunlight to electricity. The salt can be heated to 600 °C, but at the top of the tower, temperatures

above 1000 °C can be reached; problematically the salt decomposes, losing its chemical structure above 600°C. Additionally, currently deployed salt formulations remain liquid — and thus able to flow through the system’s pipes — only above 100 °C. This means that to prevent the salt from solidifying within the system’s pipes, it must be heated to the boiling point of water at night. This consumes energy and money, unnecessarily. What if a salt could be found that remained liquid at room temperature, requiring minimal heating to remain fluid, and one that could also sustain temperatures above 1000 °C without decomposing, thereby absorbing the maximum amount of solar thermal energy available at the top of the solar tower? Such a material would greatly increase the energy efficiency of the solar-to-electricity energy transformation, thereby decreasing the overall cost of power production.

To an experimentalist, this is a thoroughly daunting task because, based upon whatever chemical characteristics are available in the literature, one would have to make an educated guess about which salts might offer the desired properties, then set up a separate series of experiments-with-controls for each possibility. But with computational modeling, von Lilienfeld not only attempts to predict desired properties directly from chemical structural, bonding and quantum considerations, but also to numerically anticipate the trends of these properties for varying the materials’ chemical composition. Bridging statistical mechanics and quantum chemistry, this field is barely two-decades old and is, by definition, interdisciplinary, involving mathematics, computer science, and chemical physics. There are but a handful of research groups with the wherewithal and knowhow necessary to fruitfully pursue this type of bottom-up computational design of materials. With experience at the Swiss Federal Institute of Technology, UCLA and NYU, von Lilienfeld is among a small group of uniquely qualified designers.

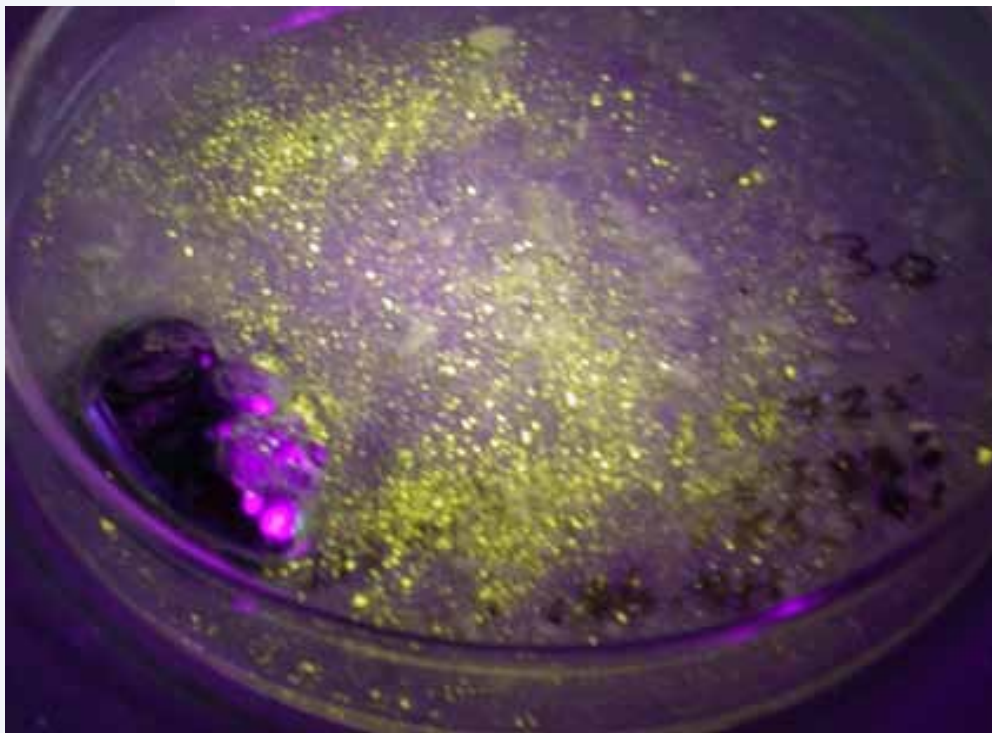
With that background, von Lilienfeld was seeking a way to pursue his ideas in a fertile landscape — with the requisite computational resources — allowing him to “focus on science,”

without the other distractions that an academic positions would impose. He communicated with colleagues at both Los Alamos and Sandia. The ability to “explore new ideas and approaches,” in

the context of LDRD funding was decisive in bringing him to Sandia, particularly against the backdrop of the “breadth of science at Sandia,” which he found “inspiring.”

The opportunity to collaborate with experimentalists has played a major role in his contentment about his position. A significant outcome of von Lilienfeld’s work is reflected in the acceptance by UCLA of his proposal to chair a three-month computer materials and bio-design workshop in spring 2011. With Sandia’s “great opportunities for collaboration,” and its “great facilities and the freedom to use them,” perhaps Anatole will continue his association with the laboratories after the completion of his fellowship, at least on some level, and he is currently conceptualizing thermal redox-catalysis that could benefit efforts to economically produce molecular hydrogen from water, or to engineer a sunlight driven reaction for approaching the issue of carbon dioxide activation to carbon monoxide for liquid fuels synthesis. This collaborative modeling-experimental approach may well set the stage for a novel solution to this key national-security challenge.

“great opportunities for collaboration . . . great facilities and the freedom to use them.”



Photoluminescent gallium nitride crystallites grown by the electrochemical solution growth method.

Skepticism without Risk-Avoidance

Learning to Grow Karen Waldrip

For someone who “back-doored” into Sandia, Karen Waldrip quickly found an oasis within a desert — from a graduate program in balmy Florida to high, dry Albuquerque and that oasis of “terrific technology talent” that she discovered working on materials science at Sandia. “Go learn to grow (crystals),” her thesis advisor recommended, and Karen ended up learning, absorbing, and contributing much more than that, nine-years later, winning a 2008 LDRD Award for Excellence for her novel method of growing nitride crystals.

Waldrip found herself awed by the attitude of that grouping of Sandia materials scientists whom she first encountered. “If you could buy a piece of equipment to do an

experiment, then we didn’t need to do that experiment,” she quips about those scientists and engineers, the attitude being that their interest was in pushing the envelope, treading into the undiscovered territory. This is exactly the attitudinal disposition that incubates LDRD idea and successful LDRD project proposals, and from the beginning, Waldrip found this attitude “exciting and admirable.”

When Karen’s research hit equipment roadblocks, she began to interact with members of the Solid State Lighting Grand Challenge LDRD, presenting bits

and pieces of her idea for growing bulk nitride crystals. All the mechanisms for nitride growth necessitated extremes of temperature and pressure within reactors, making the process slow and expensive. But Waldrip had a notion about something different, and she drew a chuckle or two from more-experienced colleagues with notions about electrochemically growing nitrides — the materials most widely used in light-emitting diodes (LEDs) for solid state lighting — at lower temperatures and pressures.

“Everyone was skeptical, but they didn’t say, ‘don’t do it,’” Waldrip distinctly recalls. A few months later, she grew the second largest nitride crystal in a test tube at atmospheric pressure. Certainly, the crystal was imperfect, but it demonstrated proof-of-principle.

As might be expected, there were job offers from private industry as well as from Los Alamos National Laboratory, but Waldrip saw the latter as a bit too long-term

and theoretically driven. It was Sandia’s engineering and electrochemistry expertise that turned her toward the Power Sources Technology group and therefore retained her as a Sandia asset. Above all, she saw the opportunity to learn more electrochemistry from a diverse and highly skilled peer group.

She found advice and management support from The Science Technology and Engineering (ST&E) Strategic Management Unit. They pointed Waldrip toward LDRD and the Seniors Investment Area. This collection of senior Sandia scientists liked her idea and provided late-start seed funding in 2004–2005, then extended it for a second year.

This initial funding gave Karen the opportunity to change the opinions of the nay-sayers, allowing her to demonstrate possibility. And it acclimated her to the notion that LDRD funding was indeed aimed at ideas and projects such as hers, which were treading that leading edge, looking out from the terra firma of “the what is” to the sometimes misty horizons of “what might be,” encouraging the risky path.

“LDRD allows you to pursue new ideas, to go where it takes you; see what’s possible.” Nor does Waldrip see any discontinuity between Sandia’s past — its weapons underpinning — and this futuristic view of evolutionary novelty. “So much spinoff technology comes from the weapons program,” she notes, perceiving the vast ingenuity that has been required to design, maintain, and modify weapons components.

Outside agencies have added their recognition of Karen’s work to the LDRD award. Her proposal to the National Energy Technology Laboratory (NETL) was ranked number one in the agency’s entire portfolio in 2007, and it funded her work subsequent to the LDRD project’s ending. Funding has also come from the DOE Office of Energy Efficiency and Renewable Energy (EERE) in the area of power electronics.

Karen is, however also incubating several new ideas in pursuit of her research goals, and she is, in turn, floating several new LDRD proposals in pursuit of these innovative notions. She notes that about 1% of total global energy expenditure is currently invested in ammonia production for soil fertilizers. In her mind, this astounding figure demands a broader examination of this chemistry, and she sees Sandia as positioned to pursue this challenge, which, in an era of energy shortages, is clearly an important national and global consideration.

In the meantime, a “quite promising” partnership appears to be evolving between GNOEM

Systems, a Bay Area startup, and Sandia in the area of crystal growth, with GNOEM’s intentions, for the present, to supply the industry with substrate wafers, and the partnership making great advances. And looking back at Karen

Waldrip’s initial “back-door” entry into the Sandia research community, one marvels at how much her mandate to “learn to grow crystals” has ramified into a lush garden of new growth opportunities. From the initial support and mentoring by experienced Sandians to the prescience of her first funding by the Seniors Council, to her award-winning LDRD project, the return on those investments for both Sandia and the nation is quite evident. And the growth and ramification of her career at Sandia has been illustrative of how LDRD investments can tender crucial support for ingenuity — even in the face of skepticism.

“LDRD allows you to pursue new ideas . . . see what’s possible.”

MID-CAREER

Establishing Bio-Nano Credibility

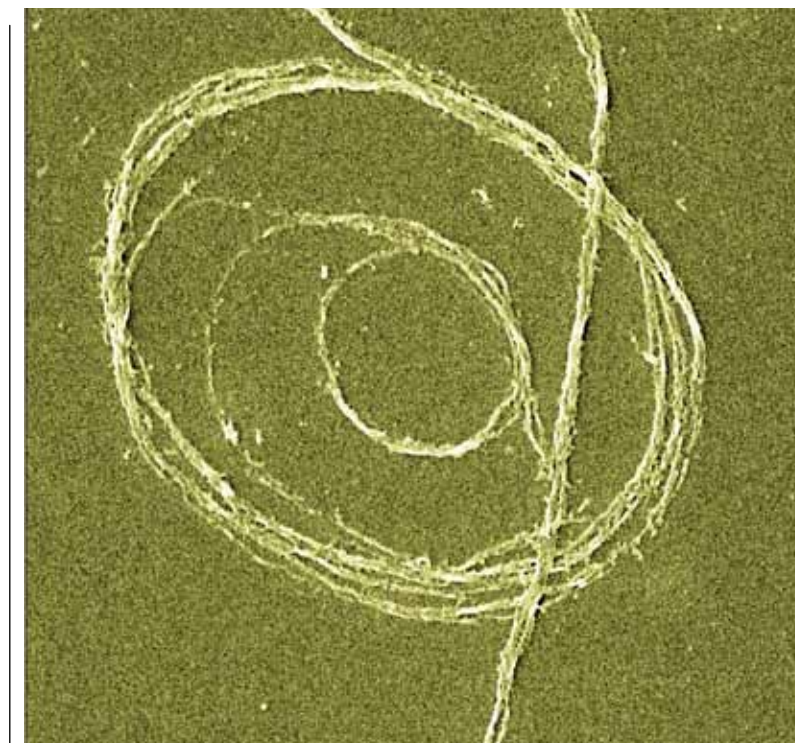
Nanomotors from Nature

George Bachand

One of the most exciting areas of research endeavor for Sandia and its LDRD investments is undoubtedly the intersection of biotechnology and nanotechnology, and George Bachand has been working at that intersection for a good portion of his career. Viruses are certainly one of Nature's most-efficient examples of nanoengineering, and coming out of a background in plant virology, Bachand, was, from the beginnings of his career, interested in the question of how biological nanosystems could play a role in engineering new nanotechnologies.

Proffering the view that Sandia is "a well-kept secret," (p. 10), Bachand was fortunate to have attended a seminar discussing some of Sandia's nanotechnology work. This serendipitous event piqued his curiosity, and after an exchange of information, Sandia offered him a staff position in 2001. His expertise immediately became invaluable on some LDRD projects involving surface functionalization of biological molecules. During a stint as a research associate at Cornell University, Bachand had become interested in biological motors, fascinating proteins that, powered by cellular chemical energy (ATP catalysis), can perform mechanical work while attached to other biomolecules, thereby exerting a nanoscale force to create motion inside or outside cells.

"It was quite a relief to not have to write a 30-page proposal," Bachand says of the LDRD submission process, one that allowed him to "learn the craft of how to write successfully" (see also page p. 40) while working his way into mission-relevant projects at Sandia, by first serving on the projects of others until he felt prepared to move into the role of principal investigator (PI) on an LDRD project. Ultimately, his work on a team studying the



Scanning electron photomicrograph of an ring-like composite nanomaterial consisting of biological microtubules and semiconductor nanoparticles (quantum dots).

utilization of biomotors for the assembly of functional nanocomposites made the cover of *Advanced Materials* in December 2008.

Bachand has been PI on a number of LDRD projects aimed at the accrual of knowledge on motor protein applications in nanotechnology, and he has gradually integrated his work with collaborators outside Sandia, under the umbrella of the Sandia-Los Alamos Center for Integrated Nanotechnology (CINT), so that they can ultimately be used in fully integrated nanosystems in a multitude of national security initiatives. The best-studied motor protein, of late, is a motor known as kinesin, which ports material inside cells, moving along nanodimensional tracks called microtubules. For example, when measured from the cell's main body to the end of it longest nerve fiber, some nerve cells in our bodies may reach lengths of two feet or more, and to move materials from one end of a cell to another requires rapid motion by these kinesin

motors. Bachand's studies entail a variety of combinations of these biological components with light-generating nanocomponents such as quantum dots (QDs). By analogy, in certain fish, these motor-track combinations move bio-pigmented crystals around inside cells, changing their local concentrations within a fish's skin to effect color changes and camouflage.

There are clear national security applications of these systems in areas such as active

camouflaged clothing for the military (where the clothing would respond to changes in surroundings by automatically adapting its coloration), as well as in ultraminiaturized sensor technologies, in which the assembly of miniature components on the nanoscale would greatly benefit from the use of biological motors.

"Sandia showed a commitment and interest in this area," Bachand points out, and LDRD provided a vehicle for him to gradually

develop projects based both on his existing expertise and new expertise that he acquired by stretching into novel areas related to those he brought with him to Sandia. As a result, DARPA engaged George in a multi-year project that ultimately involved a partnership with the Naval Research Laboratory, the University of Florida, Albert Einstein College of Medicine, and the Swiss Federal Institute of Technology.

"We wouldn't have been positioned well if LDRD hadn't given us a track record in this area." Echoed by others (pp. 27), this "track record" theme is an important LDRD outcome.

Additionally, there was a great degree of student involvement in Bachand's research, with students using the experience to catapult them into their own post-baccalaureate experiences. Bachand describes one such student whose research experience "set

her apart from the crowd," in obtaining her acceptance to the University of California at Berkeley graduate school, a prestigious molecular biology program. Another of Bachand's undergrads gained acceptance as a medical student at Johns Hopkins School of Medicine, again, a top-flight medical program. Training students "has always been a passion of mine," Bachand admits, and he praises the CINT model as a great mechanism for both developing ideas in nanotechnology and a vehicle for both researcher and student development.

Recently, Bachand has expanded his work with QDs into an LDRD-funded study of nanotoxicity, that is, investigating whether or not QDs and other commonly used engineered nanomaterials such as carbon nanotubes have significant biotoxicity. Given the growing spate of initiatives proposing to use these components both experimentally and therapeutically (drug delivery) in humans, and which are already incorporated in certain products such as sunscreen, such studies are essential to assessments of human and environmental impact.

With the expanded focus of his research into arenas that include health considerations for both individuals and population — clearly national security issues — Bachand is expanding his research funding horizons beyond LDRD and DOE's Office of Science. Although he recognizes the National Institutes of Health (NIH) as a "tough sell," he is among a growing cadre of LDRD-funded researchers who are entertaining NIH funding as a genuine possibility or reality.

Clearly, staff members like George Bachand do not perceive any funding stream as unattainable, but rather perceive Sandia, through its LDRD program and follow-on funding, as continuing to make inroads into both the fundamental mysteries of cellular function and the pathways by which biological nanomachines can be employed as genuinely integrated nanotechnologies with those

designed by human engineers to accomplish futuristic outcomes that once were considered science fiction.

An Entrepreneurial Test-Flight Returns to Sandia

Among a Cadre of Experts Mary Crawford

Solid-state lighting (SSL) — beyond the LEDs in our nearly ubiquitous cell phones and mp3 players — is the promise of lighting homes, office buildings, city streets, and even Olympic venues. But to do so requires a fundamentally deeper and more-comprehensive understanding of the semiconductor materials of which these devices are composed. And beyond simply lighting, the potential applications of these semiconductors in other electronics and optoelectronics areas are plentiful: non-interceptible, short-range communications, biological and chemical threat detection.

Recently asked to write a review of the field, Mary Crawford, at mid-career, has become a prominent figure in the optoelectronics materials science community, and she is enthusiastic about applauding the role of LDRD support in the development of her career. First and most directly tied to Sandia's LDRD mission for DOE, she is clear about LDRD as "one of the few avenues for doing higher-risk work," and based upon the uncertainty factor and the potential benefits from optimized SSL, the optoelectronics of semiconductor materials is an excellent example of high-risk, potentially high-payoff research. In general, the corporate arena will not or cannot engage in this type of risk. But having spent two years on entrepreneurial leave, Mary has a first-hand perspective on this corporate-risk topic.

"Companies appreciate us doing the farther-out work, which they can't or won't do because



White light (center of photo) produced by the mixing of light from multicolor LEDs (photo courtesy of Professor E. F. Schubert).

it could adversely impact their reactors or interrupt their product line," Crawford observes. And in the SSL arena, companies such as Philips Lumileds have been "engaged from the beginning," following progress and at times, partnering on some of Sandia's SSL R&D. This ideal partnership — in which for-profit lighting manufacturers remain continually engaged with their national-laboratory colleagues is made far more fruitful, as Crawford suggests, by the fact that the LDRD program adheres to its mission mandate from DOE to pursue high-risk research at the leading edge, a fact often ignored or overlooked by LDRD critics, who sometimes incorrectly analogize high-risk research as akin to "playing in sandboxes." Nothing could be farther from the truth in Mary Crawford's opinion.

Moreover, beyond the high-risk science, the LDRD legislation includes a mandate to maintain the vitality of the laboratories, one implication being to develop and retain staff. On this point, Crawford is equally clear: LDRD funding has allowed her to pursue science that captivates her interest, and stimulates her creativity. It has also fostered the development of an entire spectrum of her personal capabilities that have allowed her to grow from a postdoctoral research associate in 1993 to a productive, respected member in

“ . . . how a new staff member learns to write proposals, bring together a team, and present his or her ideas . . . ”

her field, who attracts invitations to author articles and consult on new initiatives. For LDRD is very much, in Crawford's view, “how a new staff member learns to write proposals, bring together a team, and present his or her ideas” to peers for review and scrutiny. Soon after her first stint as principal investigator on an LDRD project, she was asked to become a thrust leader for a portion of the extensive and successful MicroChemLab™ project, to develop a compact, short-wave vertical cavity surface emitting laser (VCSEL). “It was the first time I was directly exposed to such a diversity of folks in other fields,” she recalls. It required her to formulate presentations to upper management that encouraged cross-disciplinary collaboration, and spurred her to take the risk of entrepreneurial leave, as senior scientist and director of R&D for a small startup. And in some sense, her LDRD research experience both facilitated and permitted that path. “I had no concept of what it was like to work in a corporate environment,” she observes, and the experience provided “perspective on the cost-savings and yield,” production aspects that companies — especially small ones — must attend to.

“Many companies, especially start-ups, can't support advanced modeling capabilities,” Crawford also emphasizes, commenting on the astounding capabilities of a laboratory like Sandia, where a great percentage of LDRD projects include both experimental and modeling/simulation initiatives in parallel.

Nor does Mary underplay Sandia collaborations with academic partners. “I always wanted to collaborate with him,” she says of Rensselaer Polytechnic Institute's (RPI) Professor Fred Schubert, a pioneer in optoelectronics. She credits the national laboratory-academic partnership, National

Institute for Nanoengineering (NINE) as one of the avenues to that collaboration, its educational emphasis important to her, as she now finds herself at a point in her career where she derives great satisfaction from mentoring young researchers. “LDRD is a great vehicle for early-career development” and “a great way to get postdocs involved in research.”

Echoing the comments of others (pp. 23 and 27), Mary comments on the way LDRD-funded projects “lay the groundwork,” paving the way for funding from DOE's Office of Energy Efficiency and Renewable Energy (EERE). “We write proposals with credibility,” she asserts, because the record of scholarly publications and presentations deriving from LDRD projects establish that expertise and agencies such as EERE and DARPA “want to see some proof of concept” before they will fund follow-on work. And beyond LEDs, Mary sees smart lighting, with communication aspects such as lights that permit two-way communication interactions with emergency vehicles and even more-remarkable applications of her work — such as probing and manipulating (for sleep and health benefit) human circadian rhythms — as future horizons to be investigated.

“I'm so spoiled, here,” Mary reflects, commenting on the availability of expert-level peers in other fields at Sandia; “if I don't know something, I go to a Ph.D.-level expert at Sandia. Companies don't typically have that degree of staff diversity.” That commentary focuses a telephoto lens on the value of a national laboratory like Sandia — particularly its cutting-edge LDRD Program research — for US competitiveness in the global marketplace. As recently emphasized by the president, the United States must regain that global leadership, and it is that corporate-national laboratory-academic partnership that can lead the way. By helping to develop the careers of researchers like Crawford, the LDRD program is helping to ensure that the

return to US global S&T preeminence can become reality.

Gaining Preeminence in Clean-Water Initiatives

Collaborations in Pursuit of a Global Challenge

Randall Cygan

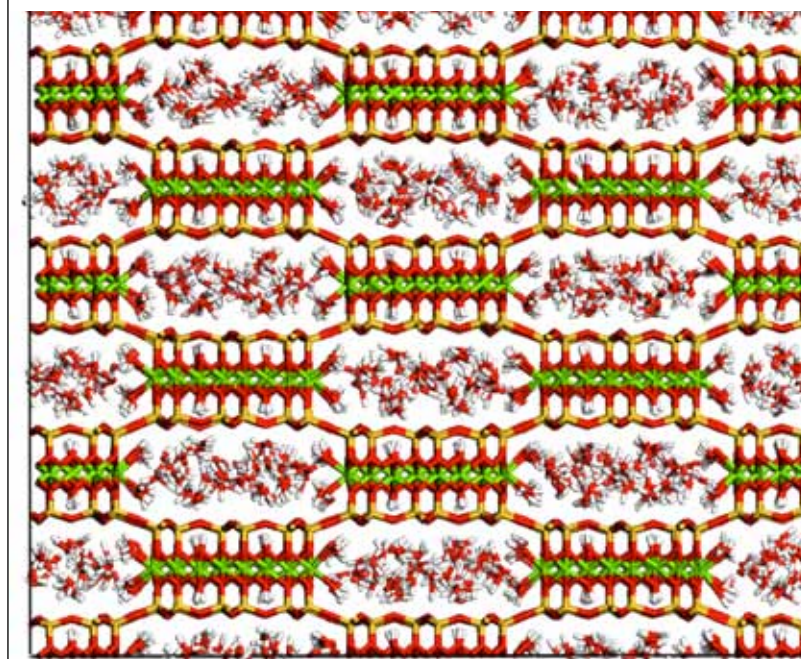
“Water water every where . . . but nary a drop to drink.” This misquote of Coleridge's *Rime of the Ancient Mariner* has been, lately, more prophetic than anyone would have imagined. For on a living planet whose individual organisms tend to run to compositions of about 70% water, by weight, much of that water has become — or was already — contaminated by dissolved substances such as metal salts. This is less of a problem for certain plants, bacteria, and fungi, which possess varying degrees of “salt-tolerance,” but for humans, potable water, that is, suitable for consumption, must be relatively free of heavy metals and certain organic contaminants, but also cannot contain significant amounts of what might be considered relatively harmless dissolved salts such as table salt, sodium chloride.

Most people recognize that we cannot live by drinking seawater, the problem being osmotic pressure. The end result of this disparity is that our tissues actually lose water to seawater, by osmosis — the net result, dehydration.

To become potable, seawater and the large number of worldwide underground aquifers, which often contain expansive water supplies, must be desalinated — reduced in salt concentration. And with the ever growing planetary disparity between supply and demand of potable water, the issue of desalination/purification of these water sources is a growing concern. Hence, quite understandably, Sandia LDRD has funded a number of cutting-edge approaches to

desalination technologies, and, for many years, Randall Cygan has been a leader in pursuit of understanding the fundamental science underpinning the interaction of water and salts with other materials from which desalination membranes are constructed (reverse osmosis [RO] membranes are one example). What distinguishes Cygan's career is not only his dedication to the science, but also his ability to pursue new directions while establishing collaborations focused on finding solutions.

In Cygan's case, such collaborations have not simply manifested as by magic; instead, he has created space for them in his career in several ways, most notably by the willingness to accept the challenge of applying his scientific expertise in a new field such as environmental physical chemistry, and by increasing his understanding of potential collaborative endeavors, such as by expanding his knowledge of biotechnology through course work at the University of New Mexico. With funding from the Office of Basic Energy Sciences and LDRD, Cygan has translated this combination into a career rich with rewards. About a decade ago, an LDRD Office-Harvard University



Structure of water molecules in the nano-sized channels of a zeolite-like material as obtained from molecular dynamics simulation.

“*It all came out of LDRD . . . they would have walked away if they hadn’t seen the scholarly publications from Sandia.*”

collaboration put him in contact with an environmental study — using atomic force microscopy — examining limestone (calcium carbonate) dissolution and its effect on monuments, both of antiquity, such as Mayan ruins, and of US culture, such as monuments in Washington, DC. Because this entailed a foray into quantification of the action of bacteria, this constituted a stretch into the life sciences for Cygan, and marked a new funding niche for his future work, namely environmental chemistry.

Part of the impetus for this Harvard-Sandia interaction was the Sandia Campus Executive Program, funded through the LDRD Office’s Strategic Partnerships investment area. Cygan applauds this program for its benefits in helping students, promoting collaborations with faculty, and helping move his own career in new directions. A subsequent Campus Executive–motivated collaboration with University of Notre Dame brought five years of funding for an environmental molecular sciences initiative studying fundamental processes entailed in molecular contamination of soils, with bacterial processes again at the forefront. This brought Cygan additional experience and expertise and, moreover, allowed him to apply his knowledge of vibrational spectroscopy to zero-in on water and its interfaces with other materials.

Such interfacial water studies became the focus of a large LDRD project, with numerous Sandia staff involved, and of which Cygan served as one of four technical leads. The project initially assembled a workshop on the topic, drawing about 60 participants, a select group of whom became collaborators in the interfacial water LDRD. Now becoming established as a leader in this area, Sandia’s water initiative drew additional funding from Congress. Subsequent collaborations eventuated with the Bureau of

Reclamation and with the University of Illinois’ (UI) National Science Foundation (NSF)-sponsored “Water CAMPWS” (Center of Advanced Materials for Water Purification of Water with Systems).

“It all came out of LDRD,” asserts Cygan about this fruitful collaborative work; “they would have walked away if they hadn’t seen the scholarly publications from Sandia.” A memorandum of understanding (MOU) now exists between UI and Sandia, and according to Cygan, the water CAMPWS “sees Sandia as representing DOE and the National Laboratories” in water issues. Cygan also credits Senior Manager John Merson for recognizing the need for a scientific underpinning to examine the fundamental issues in membrane technologies, without which science it would be difficult, if not impossible, to improve the technologies. The key issue here is energy efficiency: since it requires energy to move salinated water through nanostructured membrane water-selective pores, a deeper scientific understanding may enable the fabrication of materials that will require a lower energy expenditure during desalination. Add the problem of membrane fouling through biofilm formation, that is, growth of microorganisms on the membrane surface, and one begins to appreciate the scope of this challenge.

“We need fundamental science, and we need it now,” says Cygan, whose 2008 LDRD Award for Excellence attests to the quality of his work during a career progression that has led him to a position of major player in a field that was once possibly not even on his list of science-career choices.

Modeling — and Managing — from Petroleum to Proteins

Seamless Transitions Grant Heffelfinger

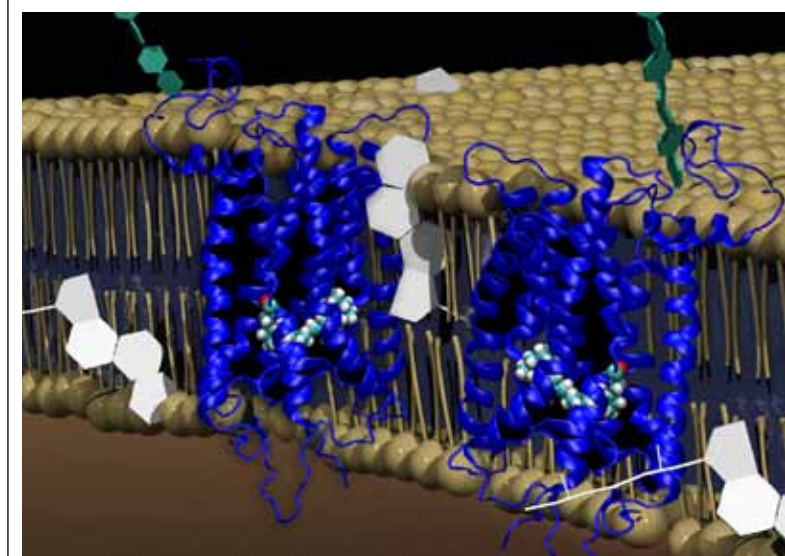
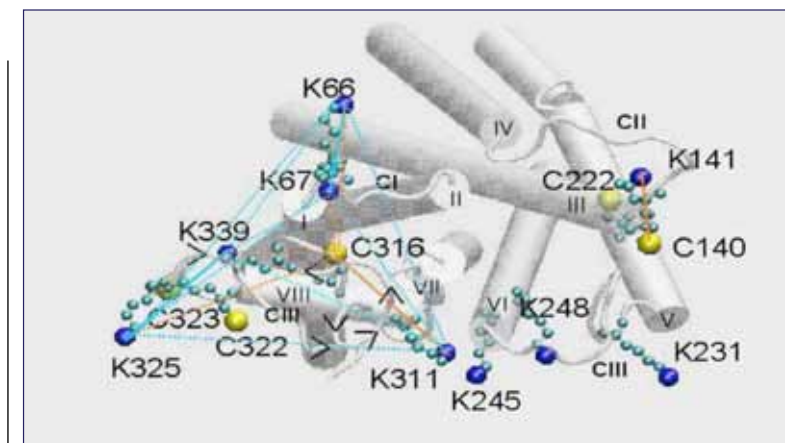
From the computational modeling of the chemical physics of fluids to the Sandia biofuels initiative — such is the scope of the scientific

transition encompassed in the Sandia career of Grant Heffelfinger. Moreover, in reflecting on what might seem to be twists and turns, but what really feels more like a smooth, evolving flow, Heffelfinger is unrelenting in his praise of LDRD funding as the transitional facilitator: “If you look at my career path, I wouldn’t be here . . . or wouldn’t have done what I did without LDRD.”

Arriving at Sandia as a resource for petroleum chemistry, in an initiative investigating oil and gas storage, Grant discovered LDRD almost by accident. This portal into LDRD funding allowed Heffelfinger to consider the possibility that his background, indeed his doctoral work building software codes for molecular dynamics, could be valuable in support of several Laboratory missions involving gas storage and absorption. He developed a code that modeled molecular diffusion under conditions of a chemical potential gradient through macromolecular assemblages, for example, membranes for separating racemic mixtures and drug diffusion through biological membranes. These molecular-dynamics modeling initiatives became cooperative efforts with industrial partners, such as DuPont and Bristol Myers Squibb, and ultimately led to the LADERA variation of the LAMMPS molecular dynamics code, released by Sandia (and updated regularly) into public domain. Some of the simulation work involved aging of components in weapons systems, a key aspect of stockpile stewardship.

With Grant’s background in writing code for the precursors to massively parallel computers, the advent of the ASCI project provided another opportunity for career development. In this instance, Heffelfinger’s experience made him a logical candidate for a position as founding manager of the ASCI computational material dynamics program.

During the late 1990s, his Grant’s path inexorably forked into the life sciences, as interactions with academia were received by



Structural model of the protein, rhodopsin, alone (top) and in the context of a biological membrane (bottom), its functional environment.

Sandia upper management as the signal to seriously plunge into life science research. With his material dynamics modeling expertise, Grant became one of three logical department managers to manage this effort in the materials dynamics of biological systems.

“LDRD was the cradle that nurtured this initiative,” Grant unambivalently offers. With clearly, no track record, and hence no readily available funding from other sources, including the Office of Science, it had to be LDRD that would gestate a biosciences capability for Sandia. The payoff was rapid and significant — a \$36M project (\$18M to Sandia) to participate in the human genome initiative with Celera Genomics, and an ambitious project to utilize the complete genomic information of oceanic

“LDRD was the cradle that nurtured this [biological sciences] initiative.”

carbon-fixing cyanobacteria (blue-green algae) to generate a deeper understanding of the metabolic processes in this key component of phytoplankton — the base of the aquatic food

web that removes carbon dioxide from the oceans and transforms it, via photosynthesis, to carbohydrates and fats (including oils). Sandia’s current leadership in the initiative to utilize such algae as a potential source of oil-based transportation fuels (while recycling carbon dioxide, CO₂) is an offspring of that initial project.

More importantly, Grant and several of his collaborators perceived this Sandia transition as a wave that Sandia simply had to catch and ride, its surfboard the incredible parallel capability in molecular dynamics simulation. And LDRD was right there, exactly where it was supposed to be — at the cutting edge — making investments in parallel computing and facilitating this capability, which is so crucial to understanding the complexity of both individual proteins and the molecular networks that regulate biological processes. Grant’s prior work in gradient-driven diffusion through membranes, in addition to other aspects of his work, was now, immediately applicable to gradient-driven diffusion through the semipermeable membranes of living cells. And although DOE Office of Science funding from the Genomes-to-Life project would be forthcoming, LDRD investment preceded that funding, keeping the initiative elegantly balanced atop that wave. Both modeling and experimental aspects were funded, including the first applications to the life sciences of Sandia’s hyperspectral microarray capability. (p.40)

For Grant Heffelfinger came the logical request from Sandia upper management to assist in managing the Sandia biofuels initiative, a task in which he is currently engaged. This represents a transition from the fluid dynamics

of storing Nature’s “ancient sunlight” gas and oil to understanding and enhancing the molecular dynamics of newly synthesized, Sunshine-to-Petrol oils made with genetically and proteomically engineered algae (among other projects). In overview, the transition seems like a logical one. But to smooth that transition, to create a logical flow from one arena to the other, LDRD was there with seed funding to allow the testing and actualization of the ideas required to assist a staff member in developing and enhancing necessary pieces of expertise.

And interestingly, Grant is able to step back and see the entire landscape. Noting that LDRD funding has assisted in allowing Sandia to hire more scientists with a depth of experience in molecular and cellular biology, Grant reflects, “as the Laboratories’ biology effort matures, I expect that there will come a time when someone will replace me for the biofuels initiative, and I’ll move on.” Undoubtedly LDRD will be there to facilitate those transitions, as well.

Seeding New Algorithms and New Careers in National-Security Surveillance

The Opportunity of Blind Alleys Katherine Simonson

How does a doctorate in statistics translate into multiple successful Sandia LDRD-funded projects with definitive national-security impact? Such an interesting and seemingly unusual progression frames the career path of Katherine Simonson. During an approximately twenty-year career at the Laboratories, Simonson’s work has exhibited a fundamental ingenuity that characterizes successful LDRD endeavor, and its collaborative scope has impacted the careers of several other scientists.

It is no secret that persistent surveillance and reconnaissance is conducted by the US, its allies, and its adversaries. And given the multiple

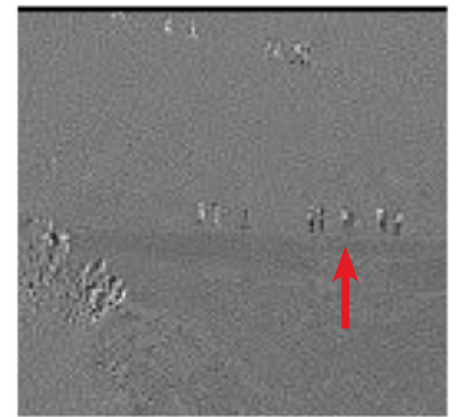
10-Aug-2007, 10:55:22 am



10-Aug-2007, 10:56:29 am



Difference Frame, Registered



With proper image registration, results of scene subtraction of the same scene at two time periods about one-minute apart, shows the appearance of new features in the scene, such as a number of people standing along a road on a ridge (indicated by the arrows).

forms of national security threats, improving the accuracy of such surveillance becomes critical. But the myriad types of sensors that survey the environment and relay information to intelligence analysts suffer from a variety of limitations that are currently best dealt with by devising superior image-processing algorithms. Such algorithms can compensate for various sources of noise and other effects in the collected images, such as “jitter,” which generally denotes deviation or defect in a digital signal, displacing that signal from its ideal position in time or space, and therefore, causing artifacts in the signals arriving from sensors.

Such problems are amenable to statistical analysis, and for a statistician arriving at Sandia, Simonson experienced an immediate “excitement about the diversity of work ongoing.”

Beginning in Sandia’s Statistics group, she moved on to apply her skills to radar target recognition with a team developing and refining algorithms for synthetic aperture radar (SAR) data. It was at that time, almost a decade into her participation in Sandia programmatic work, that she applied for her first LDRD funding, but was unfortunately unsuccessful. But the attempt itself was indicative of the germination of new ideas. Simonson perceived that what was lacking was

an entirely novel — and global — approach to improving sensor-generated data.

Ultimately, Simonson persevered and received LDRD funding for a proposal involving improved geolocation from space-based sensors. The statistics-based technique developed under this program enabled a new, higher-precision, edge-based method, predicated on the premise that algorithms must be able to provide a measure of the statistical uncertainty associated with their solutions, and therefore, be able to recognize poor solutions. This prevents errors from propagating, meaning that the probability that images would reveal artifacts, such as due, for example, to the same monitored scene experiencing weather changes (as from a sunny to a cloudy day), was greatly reduced.

Another funded LDRD project stemmed from the observation that so-called staring radiometric sensors — those constantly monitoring environments to detect changes in electromagnetic radiation (visible and other light) — required advances to compensate for artifacts in detection of changes in scenes, arising from sensor platform jitter. Analysts needed to know some estimate of the confidence — or lack thereof — that the features of the scene detected as differences were actually significant, or were, instead due to jitter-induced artifacts. The challenge was

“*What a great experience for a graduate student . . . it’s fun to watch them take ownership of their work.*”

to develop algorithms that could tell an analyst what they “knew” and what they didn’t.

In the intelligence arena, “false alarms” caused by jitter or by weather changes constitute a significant problem. And perfect rapid-fire precision is extremely computationally intensive. Simonson’s current LDRD project pursues a statistical approach combining both temporal and spatial variation to weight each pixel in an image. The result is a much better measure of scene changes, at a lower computational cost, which also reports fewer false-alarms. And the algorithm knows what it doesn’t know; if its solution in

a particular case is not a good one, it reveals that fact to the intelligence analyst.

This algorithm appears to be generalizable to different sensor systems, and a patent application for the methodology has been submitted. A co-author on that patent and on a paper in preparation is Tian Ma, who was born in China and moved to the U.S. at age 11. After obtaining his MS at the University of Illinois, Ma has “really blossomed” at Sandia, according to Simonson. And a prior publication, included Steven Drescher as an author, a Sandian and UNM graduate student who found his MS thesis topic within his work with Simonson. She sees this mentoring of students and new staff as implicitly encouraged by the LDRD process. “What a great experience for a graduate student,” she observes; “it’s fun to watch them take ownership of their work.”

As this sensor-algorithms program continues to grow, earning outside funding to solve special types of detection and tracking problems, Simonson reflects on an important point regarding the value of LDRD projects in her career. This is the issue of blind

alleys, which in an LDRD project, can be opportunities. Three months into her first LDRD, she saw that what she had proposed was not going to work, that she would need to abandon the approach. But the right turn that she took at that point turned out to be a boon, leading to a more-powerful approach that could solve more-difficult problems, one with greater overall programmatic impact.

Simonson is unabashed in her praise of the LDRD process as responsible for significant improvements in operational performance in the Sandia sensors program and a significant return-on-investment to Sandia from the programmatic funding from outside agencies, and is equally grateful for its contribution to enriching her career as both researcher, colleague and mentor.

Applying Expertise to a Breadth of Discovery

Postdoc to Project Lead

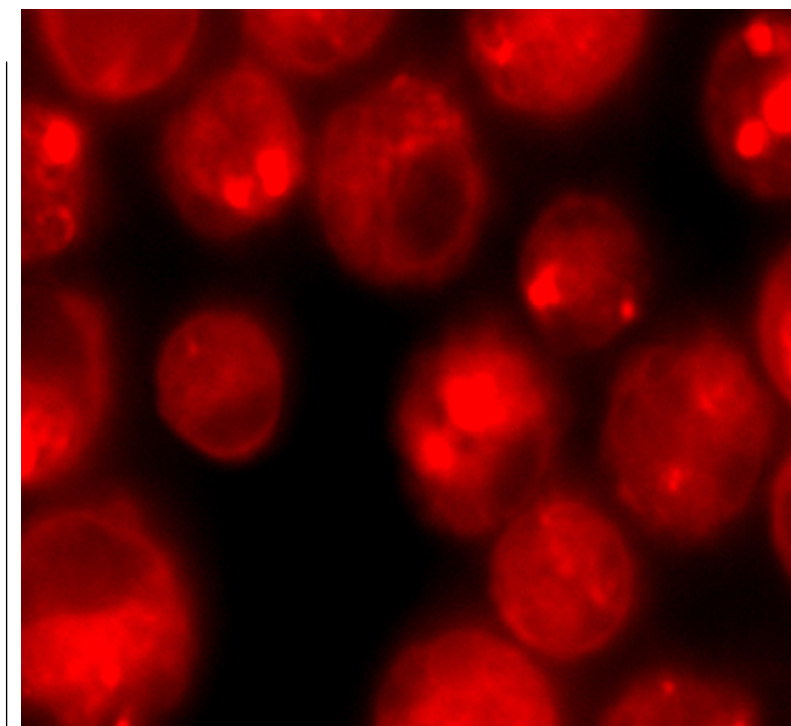
Seema Singh

A biophysicist utilizing Atomic Force Microscopy (AFM) studying the structure and function of membrane proteins — an important class of biological molecules regulating the function of living cells — Seema Singh was introduced to Sandia as a postdoctoral research associate, a 1996 Ph.D. recipient from the University of New Mexico, at a time when Sandia was seeking to expand its role in DOE’s biosciences initiative. Playing off this somewhat serendipitous connection, Singh came to Sandia, a biophysicist among chemical engineers, some of whom were examining problems with perhaps similar physics underpinnings, but in inorganic systems rather than biological ones. In that sense, Seema became a linchpin in a transition, and so from the beginning, her career investment at Sandia was marked as one both of great challenge and great potential.

Introduced to Jeff Brinker (p.38), Seema perceived several research directions that piqued her curiosity, and so, she seized the initiative and began attending the research discussion meetings of Brinker’s group in the Advanced Materials Laboratory. At the time, Brinker and his associates had begun employing proteins, such as antibodies, in the identification of mission-relevant chemical compounds, and also had begun investigations into the area of biomimetic processing, that is the synthesis of biologically inspired composites. Although not directly tied to her thesis and postdoctoral research expertise, Brinker’s research was intriguing, and Singh began to expand her focus and her expertise in the arena of powerful techniques for viewing surfaces at the atomic level with resolutions in the nanometer range. Participating in several LDRD projects during her initial years at Sandia, she also deepened her knowledge of nanoporous materials (of which biological membranes are one type).

But biology again intervened, in the person of a pregnancy, which Seema felt might compromise her full dedication to her work; so she offered to step aside for the good of the projects in which she was involved. With the birth of her son, in 1999, she departed Sandia. But the diverse and intriguing cross-disciplinary LDRD-funded initiatives at Sandia exerted their magnetism. Later, hearing that she had returned to the west, and respecting her scientific acumen, Brinker invited her to again join his research group

Singh made significant contributions to the LDRD-funded research on superhydrophobic coatings (the eventual recipient of an R&D100 award), performing all the IFM work on that project. IFM or Interfacial Force Microscopy is a variant of AFM developed at Sandia, which can measure the force between two nanosurfaces as they are separated. And in this body of research came stunning new revelations about the forces by which superhydrophobic surfaces (those that



Micrograph of triacylglyceride droplets (brightest red areas) within cells of the algae *N. oleoabundans*. Precursors to oils, such biological lipids ultimately derive from carbon dioxide and water, and their synthesis is powered by solar energy in photosynthesis.

strongly resist wetting by water) interact. Conventional wisdom about the types of chemical bonding that have always been proposed as acting among water molecules and between such hydrophobic surfaces appear to be inadequate to explain the observations obtained with the IFM. These observations suggest that the forces acting to “bond” such surfaces and deny water molecules a chemical interaction (wetting) may be acting over much longer distances than previously thought. The discovery’s importance can be measured to some extent by the degree to which it penetrated both the science and science news literature, both print and on-line, from its publication in *Nature* in August of 2006 through the following six months

But Seema’s talents were not limited to microscopy. She exhibited a good rapport with graduate students, and ultimately took charge of the postdoctoral associates in

“*LDRD projects truly shaped my future.*”

Brinker's group. And with her expertise in lipid bilayers (the structural base of biological membranes, combined with

Brinker's expertise in silicon-based materials, they collaborated on amazing LDRD-funded studies that developed artificial extracellular environments for living cells, which hold the potential for revolutionizing bio-nanotechnology, the interaction of nature's nanotechnology with inorganic silicon-based nanotechnology.

Currently, as a staff member at Sandia, California, Singh now leads an LDRD project studying the fundamental factors in promoting the secretion of oils by algae, an initiative to harvest biodiesel whose energy source is ultimately solar, through photosynthesis. Along the same lines, she serves as Division Director of Materials Science and Dynamic Studies of Biomass Pretreatment at the Joint Bioenergy Institute (JBEI), a multilaboratory-industry partnership. She also benefits from funding from the National Institutes of Health (NIH), studying topics such as nanobatteries for artificial organs. Singh also is a key player in Sandia efforts to develop biomimetic pores, equivalent to cell membrane proteins known as aquaporins that allow water to permeate them while excluding salt.

“LDRD projects truly shaped my future,” Singh clearly articulates. From a postdoc shining a beam of life science light into a purposeful crack in Sandia's institutional foundation, to a key player in a seminal chemistry discovery, to a leader in a critical bioenergy initiative, Seema Singh illustrates the creative evolution of innate talent that LDRD often supports, which nurtures and strengthens the core S&T foundations upon which Sandia builds its ever-burgeoning contributions to national security and health.

From Industry to Academia to Sandia LDRD

The Metrics of a Vision Hy Tran

After toiling in the Boston-area world of commercial high-technology, Hy Tran perceived the need for greater intellectual challenge in his life, and it initially appeared that it would be the academic world from which that challenge would come. And so, in 1997, when the offer of a faculty position came from the University of New Mexico's Mechanical Engineering Department, Tran decided that life had presented him with a rare opportunity, that is, to test the actual parameters of a vision.

In certain respects, the vision of intellectual freedom, honesty, and stimulation was, certainly, confirmed. Tran positively recalls his interactions with his students as ones of genuine satisfaction and productivity. But, in other respects, the reality of the academic world did not completely match expectation. Therefore, when the offer of a position at Sandia materialized, Tran made the difficult decision to leave that cherished academic environment — with its richness of student interaction — exchanging it, instead for a different sort of richness, that of collegial interaction, coming to an engineering environment where metrology, in the form of, for example, the Primary Standards Laboratory, had been an area of longstanding importance at Sandia. Stimulated by his interactions with colleagues, he was motivated by a question posed by one of his managers. It was a simple question: “how would you go about measuring this?”

This is a rather good and challenging question, Tran thought, researching the literature and finding that no commercial method for answering the question existed. And as he began to ponder his response, a kind of Pavlovian reaction clicked-in, one he had developed during his stint in academia. Tran logically turned to the LDRD program for assistance, submitting

an idea, which his strategic management unit (SMU) viewed as serving its interests in the context of Sandia's mission. They encouraged him to submit a proposal. Funded for two years (FY 2006–2008), the project's thesis was that the limitations on measurement accuracy for mesoscale parts — as found in many Sandia-engineered devices, including those in nuclear weapons, was not in the visual inspection tools.

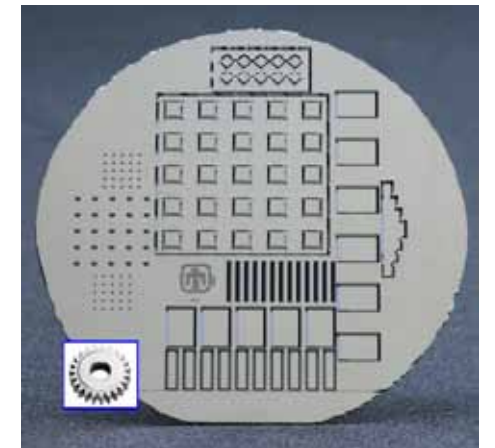
Rather, that accuracy was limited by the lack of a precision artifact, an impeccably fabricated measuring tool, the accuracy of whose dimensions could be completely relied upon. With his LDRD project funded, Tran called upon several colleagues to work with him on his ingenious idea, a premise based upon the crystal-defined fracture planes of single-crystal silicon. Using the micromachining techniques available at Sandia, the team showed that the intrinsic crystallographic planes defined by the arrangement and packing of the silicon atoms in the crystal would lead to edges that were sharp to the nanometer level. Enter Meghan Shilling, who as a graduate student at the Georgia Institute of Technology (Georgia Tech) had done significant research in edge metrology — the edge quality of mesoscale objects. As serendipity would have it, she was able to come to Sandia as technically, still a student, having defended her dissertation just two weeks before she suddenly departed for Albuquerque.

Working with Tran and Andre Claudet, Shilling was ultimately hired as a staff member, and the team used the LDRD project to show that their intrinsically defined, crystallographically sharp edges produced in silicon could engender a three-dimensional calibration structure (or artifact) enabling traceable certification of mesoscale dimensions with accuracies an order of magnitude better than before. Furthermore, silicon micromachining being a batched, parallel process led the team to estimate that they could fabricate these measurement silicon standards for ten times less than conventional artifacts.

The cleverness, accuracy, and cost-effectiveness combination was recognized by an R&D100 Award in 2008, whose submission was a bit of a spur-of-the-moment afterthought by Claudet and Tran. But aside from the great honor of the award validating the work of Tran, Shilling and Claudet, the visibility should help bring private sector partnerships to Sandia, and hopefully fulfill Tran's goal of bringing the new artifact into the broader measurement community as an adopted national and international standard. It also has the potential to extend the lives of weapons components throughout the NNSA complex.

Tran reflects, “I don't think I would've had the freedom to do this using line funding LDRD funded a hundred percent of this.” But as importantly, he is amazed by the “level of expertise” of his peers and the huge number of collaborations and professional contacts that working at Sandia has made possible, more than he would have ever made had he remained in academia. He marvels at how, in doing this piece of fundamental engineering research, his work is also impacting important goals of Sandia's national security mission.

“I love the environment at Sandia,” Tran offers, and from his perspective, a career revitalized by leaving behind one vision and adopting another, it is not hard to understand why.



Micrograph of the R&D100 award-winning artifact developed with LDRD support; inset shows a microgear from a wristwatch whose dimensions could be accurately ascertained with this artifact; such gears are sometimes used to determine brand authenticity.

“*I don't think I would've had the freedom to do this using line funding LDRD funded a hundred percent of this.*”

LATE-CAREER

Establishing Planetary-Impact Sciences at Sandia

Opportunistic Creativity

Mark Boslough

What does a scientist do with a group of creative impulses for which neither his complete skill set nor the community at large may be prepared. In Mark Boslough's case, he seizes every possible opportunity to investigate related phenomena and learn from them, with the attitude: "things that you least expect to turn into something big often do."

Boslough gravitated toward earth and planetary sciences as an applied physics doctoral candidate at Caltech. And although Mark spent a summer at Lawrence Livermore National Laboratory (LLNL), he concluded that he wanted to work at Sandia, despite the fact that no Sandian, at the time, was pursuing the type of earth and planetary science research that overlapped with Boslough's interests.

As an experimentalist, Boslough published extensively in the shock physics area. In conjunction with Randall Cygan (p. 27), Boslough was able to secure several years of National Aeronautics and Space Administration (NASA) funding, his desire to do research into planetary shock physics revived with a strongly beating heart. Enter the LDRD program. Proposing what he characterizes as a "wacky idea," Mark obtained multiyear LDRD funding to seismically model the potential effects of asteroid impacts to earth and discriminate their explosive signatures from actual weapons testing or use, a critically important national-security issue. Clearly the LDRD Office perceived the idea as cutting-edge and high-risk, rather than "wacky."

Enter comet Shoemaker-Levy 9, in 1994, which astronomers had followed with precision as its various fragments headed for collision with Jupiter. Adding to the compendium of interacting factors was the appearance of computationally savvy Dave Crawford

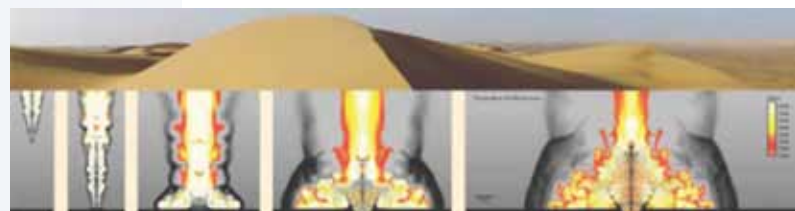


A chunk of Libyan Desert glass.

at Sandia, with interests quite similar to Boslough's and the mentoring of both men by senior scientist Tim Trucano. Boslough and Crawford had a strong notion about the plume or airburst that would accompany the comet's impact into Jupiter, publishing the somewhat radical prediction that the impact plume would be visible. The fortuitous timing of the approach of spacecraft Galileo toward Jupiter and the recently refurbished orbiting Hubble Space Telescope allowed — with a modicum of luck— the event to be observed. In three publications, the team's modeling predictions using Sandia's CTH shock physics code, were confirmed.

“LDRD set me up for these partnerships.”

“LDRD got a lot of credit, and deservedly so,” Boslough comments. The remarkable ability of LDRD to allow change of course within a mission-driven research program, such that a researcher could capture evidence not precisely specified in an original proposal, but falling within the proposal's scope was a career-changer for Boslough, establishing his reputation in planetary-impact sciences, an original goal of his career. Studying impacts of astronomical objects with earth and other planets was crucial to understanding how to differentiate their “false-alarm” signatures from those of weapons tests or actual offensive use, in order to prevent mistaken reaction



Supercomputer simulation of the progress of a low-altitude airburst.

to a space-object impact as a hostile act. By being creatively opportunistic, Boslough and Crawford seized the opportunity presented by the solar system to increase their data and check the accuracy of their models. As long as the research served Sandia's mission within the context of the original proposal, the LDRD Program allowed this opportunistic flexibility.

Continuing his career development, Boslough enrolled at the University of New Mexico (UNM). Learning how to parallelize the codes with which he worked, he ancillary learned more about climatology and saw a clear path into that area. He secured funding for several other short-term LDRD projects, one of them in paleoclimatology. LDRD thereby provided yet another opportunity for growth and partnership: looking to partner with a national laboratory, Pennsylvania State University's National Science Foundation Center of Excellence offered this partnership to Sandia, largely based on the record of computational modeling in Boslough's publications. "LDRD set me up for these partnerships," Boslough comments. Sandia was finally "in the game," toward which Boslough's research interests had been moving for two decades. A recent LDRD focused on trying to quantify the uncertainty in global climate models, drawing a somewhat ominous picture for predictions of climate-change severity, which Boslough ranks much higher than the threat from asteroid impacts. Sandia is now at the brink, as a partner with other labs, including the Jet Propulsion Laboratory (JPL) and the National Center for Atmospheric Research (NCAR) of benefitting from a large slice of funding to continue its pursuit of this research.

Meanwhile, renewed interest in high-altitude airbursts from astronomical bodies entering earth's atmosphere ensued from discovery of a decorative scarab in King Tutankhamen's tomb, which appeared to be derived from a puzzling glass whose optical properties identified it as related to glasses found in the Libyan Desert. In 1996, Boslough had written a speculative abstract about the similar origin of Libyan desert glasses as part of a meeting connected to a conference on the Tunguska event — a puzzling 1908 Siberian forest destruction. In a feedback loop between scientific research and the science media, Boslough's work — much of it LDRD-associated — came to the fore, as a Discovery Channel documentary on Tunguska invited him to present his model of a low-altitude airburst causation for Tunguska.

Nor has it been merely popular media responsive to Mark Boslough's work; the cover story paper in the March 26, 2009 edition of *Nature* featured a team that modeled, recovered fragments, and described the explosion of an asteroid in the atmosphere above the Nubian desert of Sudan, a team that included Mark Boslough. The chain of opportunity forged by LDRD's support for Boslough's creativity through the tortuous turns of his career had added yet another important link.

Developing Several Generations of Researchers at the Leading Edge

Mentoring Innovative S & T Jeff Brinker

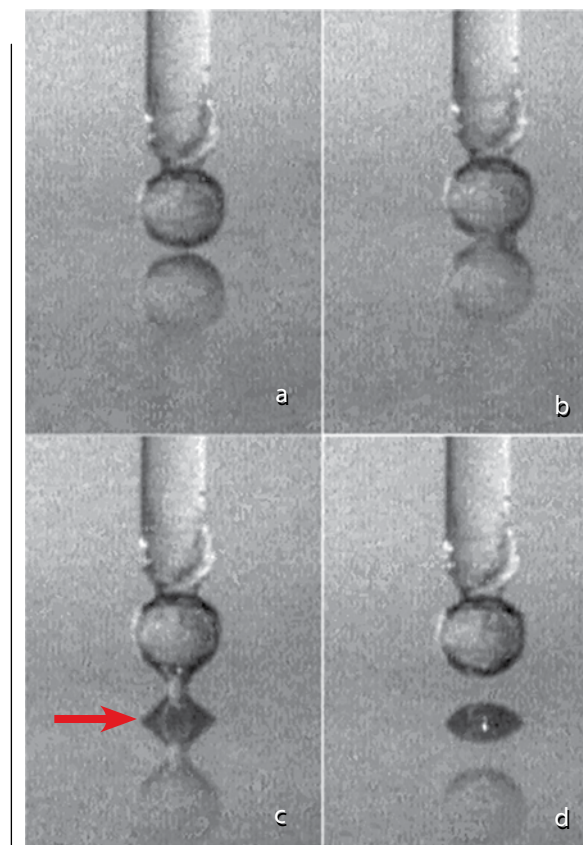
Making LDRD-funded scientific research count in duplicate and triplicate (or more) is a predominant theme that emanates from the laboratory of Sandia Laboratory Fellow, C. Jeffrey Brinker. With a simultaneous appointments as Laboratory Fellow and Distinguished and Regent's Professor of Chemical and Nuclear Engineering and

Molecular Genetics and Microbiology at the University of New Mexico (UNM), Brinker's dual appointment as an academic and a Sandia staff member and the details of his career offer a panoramic window into LDRD investments that impact staff development in a multitude of immediate and prospective ways. He and his team are headquartered at UNM's Advanced Materials Research Laboratory (AML).

Well-prepared to serve as mentor, Brinker's own career manifests a tortuous journey of successful endeavors across the natural sciences, each leading-edge evolution exhibiting the potential to make the "best of" list in popular science and engineering literature. From fundamental investigations into sol-gel physics and chemistry through coatings and other materials for sieving and sensor applications, to artificial extracellular environments for living cells, Brinker's work is truly science in the best tradition of LDRD — always at the leading edge and always seeking to evolve into new areas of potential application. He was working in nanotechnology before it was dubbed "nanotechnology," the art and science of creating materials with controlled structures and properties at the atomic and molecular levels, most palpably represented by over 20 patents.

From his roots as a ceramic scientist/engineer to his most recent probing into the Field of superhydrophobic coatings and the micro-/nano-world of cellular and molecular biology, Brinker has utilized LDRD funding to unmask a remarkable range of properties and processes. For example, his recent work plucks living cells from their customary, preferred organic environment of proteins and polysaccharides (complex carbohydrates) and transmutes their world into one of inorganic silica-and-lipid-based surroundings that simultaneously promotes the biological creation of novel nanostructures (a so-called "lithography of life"), and examines fundamental issues in biological signaling, a topic at the heart of life science.

In pursuing these diverse avenues, Brinker's list of research and teaching affiliations reads like



Successive interfacial force microscope (IFM) images in time (a through d) illustrating spherical superhydrophobic glass tip being slowly withdrawn from a similar surface submerged in water. In frame c, a cavitation called a "vapor bubble" (arrow) bridges the gap between the submerged surfaces, and forms a visual representation of the forces acting between the superhydrophobic surfaces, which are much longer-range than those predicted by standard chemical theory.

a who's-who of nanotechnology, and his ability to secure funding as an academic scientist, coupled with LDRD support for research supporting Sandia's missions enables him to leverage outcomes that might not otherwise be conceivable. At one point or another, his research group has received funding from the Department of Energy Basic Energy Sciences, the Air Force Office of Scientific Research, the Army Research Office, the National Institutes of Health (NIH), the National Science Foundation (NSF), and several industrial partners, in addition to LDRD investments. With affiliations with UNM's Cancer Research Center and Centers for High Technology

“*I have the best job at Sandia . . . I couldn’t do it without LDRD.*”

Materials and Micro Engineered Materials along with the Sandia/Los Alamos Center for Integrated Nanotechnology (CINT), Brinker is positioned to reach out into all passageways in the arena of nanotechnology, and moreover has made a rare incursion into the realm of NIH medical sciences funding for projects in nano-battery development, with potential applications in areas such as powering artificial retinas for the vision-impaired. As such he has been able to utilize this combined LDRD/external agency funding to, for example, shepherd worthy postdoctoral students through exciting research opportunities and into careers as productive Sandia staff (see page p. 32) and potential future staff (page p.10).

“Thirty years ago, when I came to Sandia, there was so much freedom to do whatever you wanted . . . as long as it was good science.” But times have changed, missions have become more focused, and budgets have contracted. Now, says Brinker, “getting mentored in an LDRD-funded project is the best thing we’ve got going for us.” Through LDRD funding, Brinker has assembled teams of researchers including Sandia staff and postdoctoral fellows and UNM graduate and undergraduate students. Brinker even manages to mentor high school students, as part of work within the education-focused National Institute for Nanotechnology (NINE), and this type of early influence upon local young people is likely to bear fruit for both the State of New Mexico and its national laboratories in years to come.

Similarly, Brinker also participates in the NSF Interdisciplinary Graduate Education and Training (IGERT) program, a unique training ground for interdisciplinary scientists (like Brinker, himself). He is continually on the lookout for fresh and interesting ideas, and is willing to promote and mentor their development. For example, when another staff

member brought current Sandia Truman Fellow, Bryan Kaehr to Sandia to present a seminar on his predoctoral research, Brinker perceived the potential for collaboration, and encouraged Kaehr to apply for the Truman postdoctoral fellowship (p. 10).

The names of UNM and New Mexico Tech undergraduates appear on several of the Brinker team’s scholarly publications, and he is clearly always looking to expand those possibilities. “The whole idea of environments like the AML is win-win,” he offers, students bringing excitement to the work, while actually cutting costs and taking their exposure to the intriguing world of nanoscience into their subsequent experiences, some perhaps returning to their roots to contribute their own acquired expertise to subsequent generations at both UNM and Sandia. In the process, their fundamental, cutting-edge research experiences with the Brinker group exhibit the potential for technological improvements of all types — from improved water-filtration membranes, to nanosensors, both inorganic and biological, to better tuberculosis vaccines and improved drug-delivery systems; and all in the context of the education of the next generation(s). “I have the best job at Sandia,” Brinker asserts, and “I couldn’t do it without LDRD.”

Teaching the Art of Scientific Proposal

Senior Scientist Mentor Dave Haaland

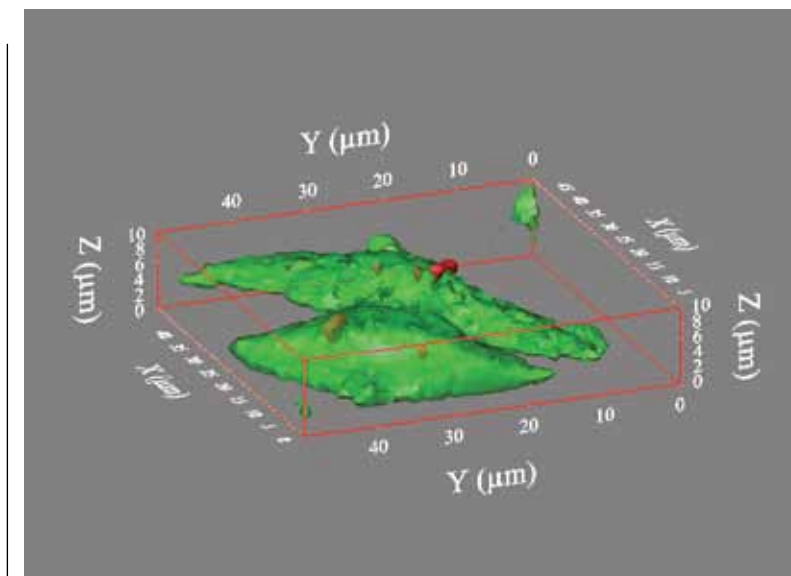
Spend the last portion of his career in biology-centered research? The thought likely never crossed Dave Haaland’s mind as a Ph.D. candidate working on low-temperature spectroscopy of organic molecules. But a Sandia career path that saw him achieve the status of senior scientist took several turns from its beginnings as a summer intern, and did, indeed, lead to his drawing his

chemometric skills into Sandia’s nascent biology initiative during the 1990s, after about 30 years of material-science R&D.

Transitioned into high-temperature spectroscopy upon his arrival at Sandia in the early 1970s, Haaland had to jump onto a learning curve almost from the first day of his Sandia career, and he never really stopped riding that curve. Similarly to Jeff Brinker (p. 38), he recalls the early days as structured so as to encourage that knowledge and skills acquisition and its application to research. For someone who had decided that he wouldn’t teach because he didn’t think he could be as good as the best of his professors, he found that the freedom to pursue creative ideas as a scientist was what motivated him: “What I really enjoyed was doing the science,” Haaland comments, Sandia research foundations providing “the engine” for his research. For a scientist, less proposal work and more time in the laboratory meant a more-rewarding work life. And it also translated into the possibility of increasing the breadth of one’s research capabilities. Haaland recalls that, for example, he was able to work with a statistician to learn multivariate analysis, which would, ultimately, become quite important to his research in combination with a hyperspectral microscope that he helped develop, and which has become a very important tool to biologists and other Sandia scientists.

From miniaturized spectrometry for noninvasive monitoring of blood analytes to multivariate analysis of hyperspectral images from satellites, to material aging, and ultimately, to immune system biology, Haaland’s own LDRD-funded projects have been as diverse as they were inventive.

Haaland attributes at least part of his success to understanding the process, soliciting feedback to his ideas, and clarifying the “dos and don’ts” of proposal writing. And his collaboration with scientists and engineers of diverse backgrounds and experience levels



Hyperspectral fluorescence image of two immune system macrophages (green) having ingested bacteria (red or reddish-brown spots).

in projects as large and highly staffed as the MISL (Microscale Immune Studies Laboratory) Grand Challenge provided both a significant audience and a significant set of interaction as Dave shifted his career focus toward biology, in many respects, a response to Sandia’s expansion of its national security mission. MISL included academic scientists from the University of Texas Medical Branch (UTMB) at Galveston and the University of California, San Francisco (UCSF), and over the course of his career, Haaland spent approximately 20% of his time in university collaborations, with an estimated 40% of his publications including an academic co-author. And graduate students have been a significant part of such collaborations. “I love mentoring students,” Haaland admits, citing the high energy and dedicated focus of graduate students as positive contributors to his laboratory over the years.

But Haaland perceives the current landscape to be a much rockier one for the beginning scientist, whom he sees a having to “hit the ground running.” Hence, a main focus of Haaland’s mentoring has been his assistance to his colleagues in securing LDRD funding. Having himself served as adjudicator on proposal-assessment committees in several different scientific areas, he characterizes

“*I love mentoring students.*”

decision-makers as willing to talk to staff members, willing to provide feedback on idea quality, and to discuss methods for improving idea focus and presentation to enhance LDRD funding prospects. Each LDRD cycle begins with a call for ideas in defined areas of Sandia's mission space, and Haaland, of course, advises applicants to “match the call with your idea submissions, as closely as possible.” He cites creativity as another key factor, that is, an awareness that LDRD is genuinely interested — and indeed charged by its founding legislation — in funding risky, leading-edge proposals, innovative science and engineering poised to have significant impact on national and global challenges. Haaland finally advises writers to present ideas and proposals concisely, to write long, but then pare down to the meat of the idea, learning to incorporate the most possible information in the fewest words. He has been rewarded by a high success rate among his mentorees, dozens of whom still pursue R&D at Sandia.

Against a career favored by research success in diverse areas — from materials science through chemometric analysis of living cells, Haaland was instrumental in the LDRD program's formation of the Seniors' Council investment area (IA). Concerned about particularly younger staff's ability to pursue creative ideas, this IA generally funds one- or two-year projects in a diversity of research areas, their worthiness adjudicated by Sandia's senior scientists. Dave comments that life is more difficult for an early-career scientist beginning at Sandia because the competition for extramural research funding is so much more intense than it was when he began his career. His hope is that seed money available through the Seniors' Council investment area might assist a beginning staff member in demonstrating the quality and viability of his or her research program, a sort of jump-start. Haaland's part in this initiative exemplifies yet

again, the global nature of the mentoring that characterized a long and fruitful career at Sandia.

Building the Most-Effective Teams

Keeping an Eye Out Dave Reedy

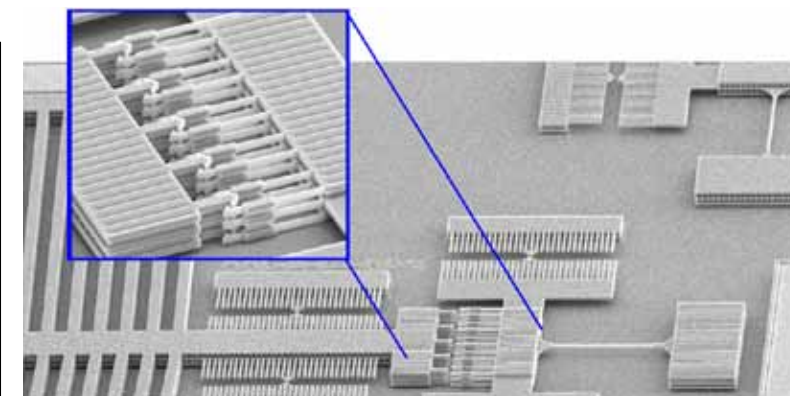
With thirty-two years as a Sandian, Dave Reedy is quick to admit his “top-five-percent” tenure status. And that exalted position has also included an early foray as principal investigator (PI) in LDRD funding, near the program's inception in the early 1990s. That project, an examination of composite material properties, published its peer-reviewed results in 1997. Meanwhile, Reedy was recruited onto several other LDRD projects, then proposed several others of his own in the early part of the millennium. He is currently PI on a proposal that examines material failure at the microscale, and a team member on another nanomanufacturing.

All in all, Reedy has been a leader or team member on 14 LDRD-funded research projects. Why? He obviously loves the challenge, particularly where it involves tying together theory and experiment. But for Reedy, the allure of LDRD research goes beyond those forays into engineering “no man's land.” For Reedy does not believe in traveling solo. “The real value of LDRD is in building teams with a diverse group of people,” he maintains.

Bomb casings to automobile components — composite and layered materials have uses that surround us on all fronts, and Reedy appreciates the engineering challenge to design and manufacture them more effectively. And although he recognizes the “top-down component in LDRD in terms of a management selection process that culls those ideas invited to write full proposals, Reedy focuses on the

bottom-up component of LDRD, which he characterizes as a “looking around” process. In other words, any individual staff member can look around and absorb the nuances of the work occurring in his or her area of endeavor at Sandia, and in doing so, can open a window into a better future, by incubating a creative idea about a new direction, or an evolutionary leap to a major improvement in that aspect of Sandia's mission. Once the idea becomes proposal, then the bridge building begins, and Reedy sees the LDRD Investment as paying for the bridges that connect Sandians in sometimes quite diverse disciplines to come together under the project umbrella. “The LDRD process allows you to identify people and find good ones,” he says. He cites his current LDRD, which diversely includes a young and vitally enthusiastic California staff member, who recently completed his doctorate, and two other mid-career staff, one an expert experimentalist, the other an experimentalist with strong design talents. “They bring a very active interest and energy, and unique skills and ambition to the project,” Dave says of his team members. “I keep an eye out for special people doing interesting things, sometimes offer to do paper reviews as a way to get to know them.” This reaching-out to those both near at hand and somewhat farther afield is a mechanism — assisted by LDRD-based teaming — for Dave Reedy to keep himself vital, to draw his significant skills, experience, and achievements into the present, and more importantly, into the future. “I'm doing work I never thought I'd be doing when I graduated,” he admits, and “I don't think things have passed me by, at all,” he delights.

Dave's field of composite materials and fracture has indeed significantly progressed and perhaps even radically changed with the advent of nanoscience and nanotechnology. Older models of material failures tend not to be useful under some of the conditions encountered when the materials being assessed for failure are on microchip dimensions — for example, 100 nanometers (one-tenth of a



Electron micrograph of the elements of an on-chip failure-test device. Inset shows the central area, where the male and female “gripper” components of the device interlock.

micrometer— an average human hair thickness is about 100 micrometers or 1000-times thicker than the 100 nanometer dimensions that Reedy and co-workers assess for failure). In addition to developing new fracture theory, the team is performing microscale testing, such as by introducing flaws into their materials, and it is even developing an on-chip strength tester that can test hundreds of tensile specimens on a single chip, as well as another novel on-chip test technique that has been used to test a thousand nominally identical micron-scale specimens over the course of a couple of days. Hence the project is both examining the fundamental nature of failure, as well as a pragmatically seeking ways to improve failure assessment.

The field has, quite literally shrunk to the atomic scale, and rather than shrinking away from the tremendous changes that these transformations have wrought, Dave Reedy has instead stepped up, using LDRD projects as a vehicle to contribute his engineering experience and expertise, while drawing new expertise from the research and his colleagues. So it is understandable that when asked about mentoring, he prefers, instead, to focus on cross-fertilization: “I learn as much from them

“*The real value of LDRD is in building teams with a diverse group of people.*”

as they learn from me,” he insists. From the earliest-career postdoctoral researcher to the most senior staff at Sandia, this co-equal enlightenment appears to permeate to the very core of the LDRD process, from initial proposal to final outcomes and project report. And given the crucially multidisciplinary nature and scope of the issues facing national science in the Twenty-first Century, this ability to cross-fertilize and synergize stands out as a significant strength of Sandia LDRD in the national and global interest.

Encouraging Project-Team Communication

Wish I'd had that Idea
Bill Sweatt



Diffraction-limited aspherical lenslets milled into the surface of a turned hemispherical dome of approximate 2-millimeter diameter, exemplifying micro-optics for applications such as micro-robotics.

In over 20 years in optical engineering at Sandia, Bill Sweatt has “seen” through a great variety of optical systems. After stints at both Los Alamos (LANL) and Lawrence Livermore National Laboratories (LLNL), Sweatt settled in at Sandia at an exciting time in his field. In the mid-to-late 1980s Sandia had begun an investigation into employing very short wavelength light (electromagnetic radiation) for chip lithography, that is the patterning of the circuitry on microprocessing chips. The proposed light would be of wavelengths less than 100 nanometers, characterized either as at the extreme short-wavelength end of the ultraviolet spectrum or at the long-wavelength end of the x-ray spectrum (soft x-rays). Ultimately the project

adopted the nomenclature, “extreme ultraviolet lithography (EUVL).” The challenges were numerous, from producing the light from a laser-generated plasma to collecting and focusing the light and characterizing appropriate chemical photoresists, the on-chip material upon which light acts to create patterns. Beginning at the program’s inception in 1992, LDRD funding of portions of the project’s task assisted several aspects of fundamental science and developmental work.

Sweatt led several optics projects during that period, including design and characterization of condenser optics to efficiently collect the extreme ultraviolet radiation from its laser plasma source. “This was perfect for Sandia,” he believes, particularly in Sandia’s leadership of a trilaboratory collaborative with LLNL and Lawrence Berkeley National Laboratory (LBNL), dubbed the “Virtual National Laboratory” (p. 45) And he characterizes LDRD as providing “essential support” during this collaboration.

National laboratory-industry collaborations were integral to the commercialization of EUVL, still a technology in the works at Intel. “We blazed a path showing that it could be done,” Sweatt says, speaking of Intel as “an excited, interested customer who really cared.” Even more important to Sweatt is the internal collaboration between a project’s principal investigator (PI) and its project manger (PM). Since EUVL, he has led numerous LDRD-funded projects as principal investigator, particularly in the arena of microholographic tagging of structures, and he has also served as project manager on several others involving design and manufacturing of high-precision micro-and meso-scale optics, such as for applications in micro-robotics. He

“... worthwhile projects can find a home within its funding process...”

characterizes the collaborative relationship between PI and PM as especially important to keeping a project moving in the direction of serving the needs of a given customer.

Customer satisfaction is a key element of the return-on-investment for Sandia. And Bill Sweatt’s career as a researcher partially funded through LDRD at Sandia is illustrative of an accretion of experiential components important to both his peers, to younger staff, and to the organization at large. Commencing with his joining Sandia as a team member on the enormous EUVL project, then progressing to his project leadership as a PI path-blazing on the engineering of the precise optical mirror technology that EUVL would require, he would subsequently move into micro-optics for novel national security applications, in all cases collaborating with diverse teams. Throughout his career at Sandia, he has remained abreast of the innovative LDRD projects in his area. “I wish, I’d had that idea,” he reflects, referring to specific projects, for example, exciting work he sees in microphotovoltaic technology for increasing efficiency of solar-electric systems, and in general, to diverse recent Sandia LDRD projects on which he has very likely consulted.

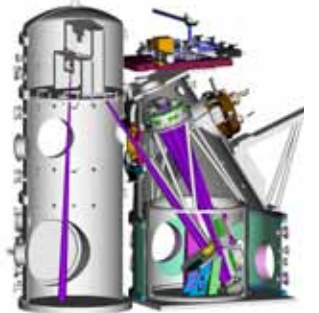
Swett’s comment reveals an aspect of informal staff-development cited by other staff members: Scientists and engineers of the stature and experience of Bill Sweatt and others like him are available to colleagues for consultation, despite the fact that their names may not, and indeed often do not, appear as participants on a given LDRD project. As expressed by several Sandia staff members and concisely articulated by nanoscientist, Mary Crawford (p. 25), “... if I don’t know something, I go to a Ph.D.-level expert at Sandia.” Bill Sweatt seems to naturally fill the role of that experienced presence, and in assuming project management for the ideas of his colleagues, he derives excitement and satisfaction from the ingenuity he sees around him, as well as a determination to be an active and interactive PM, one who fosters that ingenuity.

Sweatt sees LDRD as offering enough diversity in its efforts such that truly “worthwhile projects can find a home within its funding process.”

An LDRD Retrospective

EUVL Never Would Have Happened

Rick Stulen, VP Science, Technology and Engineering, and Chief Technology Officer



Clearly exhibiting “a sense of excitement about the future through LDRD,” Sandia Vice-president and Chief Technology Officer, Rick Stulen, also offered a window into LDRD’s past from a personal perspective.

Harkening back to the late-1980s and early-1990s, a few years before LDRD’s formal genesis (FY 1992), Stulen opined that “EUVL never would have happened, otherwise,” a reflection on LDRD’s role in supporting Sandia’s research as part of an inter-laboratory and corporate partnership leading to the seminal development of Extreme Ultraviolet Lithography (EUVL), positioned as the next crucial leap forward in the manufacture of microprocessors (the chips in computers and cell phones).

Sandia’s seminal work on the components requisite to EUVL initially spanned the period from about 1988 to 1995, a portion of that work performed in collaboration with AT&T’s Bell Laboratories. An engaged manager of that early work, partly funded in the early-to-mid 1990s by the nascent LDRD program, Stulen was later a key figure in assembling the partnerships and serving as CEO and COO of the Virtual National Laboratory, a collaboration among Sandia, Lawrence Livermore National Laboratory, and Lawrence Berkeley National Laboratory. This DOE partnership would subsequently transfer the technology under a multiyear CRADA to the Extreme Ultraviolet

Computer-generated drawing of a EUVL prototype showing extreme ultraviolet light as a purple beam generated from a plasma source at the top right-hand side of the apparatus, originally assembled at Sandia/California.

“ . . . a sense of excitement about the future through LDRD . . . ”

Limited Liability Corporation, including chipmakers such as Intel, Advanced Micro Devices (AMD), and Motorola.

All microprocessor chips are currently manufactured by lithography, in which a pattern of the desired circuitry (a so-called “mask” to

be imprinted in the silicon semiconductor) is focused — via lenses, currently— onto a so-called chemical photoresist layered atop the silicon-wafer layer. In the areas defined by the mask pattern, the light hardens the photoresist into a solid. In other areas not exposed to light, the material remains a thick liquid, which, after completion of light-exposure, can be washed away. Ultimately this leaves the

desired circuit pattern upon the silicon wafer. Two factors define the size (smallness) of the circuit elements that can be imprinted on the chip, and therefore the number of processing elements that can be crammed onto a tiny wafer of silicon. EUVL addresses both factors, but most important is the issue of light wavelength — the shorter the wavelength, the potentially smaller the circuitry features. Using an extremely short-wavelength — an order of magnitude shorter wavelength than currently used in chip lithography — EUVL allows circuit features of a much smaller size to be imprinted on a chip, which, in turn, means faster and more-powerful chips.

During the period 1992 through 1996, LDRD supported investigations into a clean, efficient laser plasma source of the short-wavelength UV radiation, as well as into both theoretical, experimental, and fabrication inroads into the development of an appropriate optical mirror system for focusing the UV light onto chip surfaces (because of absorption issues, light of such short wavelengths cannot be focused by optical lenses). The compendium of difficult physics, chemistry, and engineering challenges that such a project was compelled to illustrate the great riskiness of this endeavor, one

that could not have been pursued without a funding source such as LDRD, which Congress established to nurture exactly that type of high-risk, research.

From his vantage atop those early Virtual National Laboratory fundamental incursions into the challenges of using such a short-wavelength, high-energy light to pattern chips, Stulen reflects that Sandia “couldn’t have tapped into DOE” or other programmatically funded agency funds at the time, because of the risk aversion in those funding streams. EUVL was exactly the kind of visionary project that LDRD encourages. Although LDRD was only one of several funding sources for EUVL, its funding came at a crucial point in the project’s history, enabling progress through much-needed research into fundamental physics issues. And the project’s potential game-changing position in a realm we have all come to depend on — that of microelectronics — makes it obvious why Stulen characterizes the LDRD program as an “incredibly powerful force” capable of producing both “evolutionary . . . and revolutionary gains in skills.” EUVL remains high atop the list of forthcoming Intel chip-manufacturing technologies, with a hope that within a few years’ time, it will extend the life of the silicon chip through at least another generation of circuit miniaturization. Stulen’s other takeaway from the EUVL experience and from his more-global management of the LDRD program is LDRD’s effect upon collaboration across disciplines at Sandia, and across the potentially flimsy though sometimes daunting boundaries erected between the national laboratories and academia, and also with the corporate world. For in the consummation of the S&T possibilities of a project of the magnitude of EUVL as a potentially viable technology, the integration of a team of scientists and engineers of diverse skills is essential, and the LDRD program as a whole seeks to maintain those same values of cross-disciplinary integration and fertilization by which careers are enriched and sometimes irrevocably changed for the better.





Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

SAND No. 2009-3633P

